Reflection seismic thermometry

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LIST OF ABBREVIATIONS

- **1D** – One dimensional
- **2D** – Two dimensional
- **3D** – Three dimensional
- **AAPG** – American Association of Petroleum Geologists
- **AI** – Acoustic Impedance
- **APC** – Advanced Piston Corer
- **AVO** – Amplitude Variation versus Offset
- **BCU** – Base Cretaceous Unconformity
- **BHT** – Bottom Hole Temperatures
- **BSR** – Bottom Simulating Reflector
- **BWT** – Bottom Water Temperature
- **CCS** – Carbon Capture & Storage/Sequestration
- **CMP** – Common Mid Point
- **COB** – Continent Ocean Boundary
- **DSDP** – Deep Sea Drilling Project
- **DT** – Sonic Log
- **DVTP** – Davis-Villinger Temperature Probe
- **EOR** – Enhanced Oil Recovery
- **FGZ** – Free Gas Zone
- **FWI** – Full Waveform Inversion
- **GEBCO** – General Bathymetric Chart of the Oceans
- **GHSZ** – Gas Hydrate Stability Zone
- **GTG** – Geothermal Gradient
- **HF** – Heat Flow
- **IDW** – Inverse Distance Weighting
- **ILINE** - Inline
- **IODP** – International Ocean Drilling Program
- **K-T** – Cretaceous-Tertiary (boundary)
- **MBSF** – Metres Below Sea Floor
- **MBSL** – Metres Below Sea Level
- **MD** – Measured Depth
- **MOHO** – Mohorovic (discontinuity)
- **MSL** – Mean Sea Level
- **MTD** – Mass Transport Deposit
- **NCS** – Norwegian Continental Shelf
- **NGL** – Natural Gamma ray Logs
- **NOAA** – National Oceanic and Atmospheric Administration

- **NP** – Needle Probe
- **NPD** – Norwegian Petroleum Directorate
- **NVG** – North Viking Graben
- **ODP** – Ocean Drilling Program
- **PCS** – Pressure Core Sampler
- **PreSTM** – Pre Stack Time Migrated
- **PSDM** – Post Stack Depth Migrated
- **PSTM** – Post Stack Time Migrated
- **QTM** – Quick Thermal conductivity Meter
- **RCB** – Rotary Core Barrel
- **RMO** – Residual Move Out
- **RMS** – Root Mean Squared
- **RMSE** – Root Mean Squared Error
- **SDR** – Seaward Dipping Reflector
- **STP** – Standard Temperature & Pressure
- **SWIT** – Surface Water Interface Temperature
- **TOMOT** – Time Tomographic Inversion
- **Tpred** – Predicted temperature
- **TVD** – True Vertical Depth
- **TWT** – Two Way Travel time
- **UKCS** – UK Continental Shelf
- **VRT** – Virgin Rock Temperature
- **VSP** – Vertical Seismic Profiler
- **WBUC** – Western Boundary Undercurrent
- **WHOI** – Woods Hole Oceanographic Institute
- **WOA** – World Ocean Atlas
- **WSTP** – Water Sampler Temperature Probe
- **XCB** – Extended Core Barrel
- **XLINE** - Crossline
- **ZO** – Zero Offset

ABSTRACT

An understanding of the subsurface thermal regime is beneficial to many disciplines, including petroleum and geothermal exploration, carbon capture and storage (CCS) and nuclear waste sequestration. This project developed and tested a new methodology for determining subsurface temperature using a non-invasive approach based on the velocity information derived from seismic reflection data. By solving a one-dimensional steady state approximation of Fourier's Law, it is possible to determine a bulk thermal gradient as a function of depth, enabling the determination of temperatures across an entire volume using this methodology, termed reflection seismic thermometry. There are two principal components to this methodology, requiring 1) a bulk thermal conductivity structure and 2) heat flow and/or temperature data to condition the model. The first component uses an empirical velocity to thermal conductivity transform whilst the second uses sparse temperature data from boreholes or a bottom simulating reflector (BSR) to derive the shallow thermal regime and heat flow.

The thermometry workflow has been applied to three case studies; in the Lüderitz Basin, offshore Namibia; the Blake Ridge, offshore USA; and the North Viking Graben (NVG) in the North Sea. In the frontier Lüderitz Basin, a BSR was identified and used to derive heat flow of 60-70 mW m⁻². The Aptian source rock interval here was shown to presently be in the gas generative window. On Blake Ridge borehole velocities and a BSR were used to determine heat flow (43-56 mW m⁻²) and subsurface temperatures. Finally, methodology validation was conducted in the North Sea Basin using a high-resolution 3D full waveform inversion (FWI) velocity dataset calibrated with 141 wells. Forward models of subsurface temperatures were calibrated against the borehole temperatures, with inverse modelling used to derive heat flow at km scale lateral resolution. The availability of a fast track velocity volume for this area allowed comparison with the FWI derived thermal model results. It was found that stacking velocities were lower than well and FWI velocities, leading to overprediction of subsurface temperature. Modelling the temperature profile for CCS well 31/5-7 showed bottom hole temperature (BHT) within 6 °C of recorded BHT. With application and verification of the method in different basins, the versatility of the work conducted is demonstrated. It is envisioned that this technique opens avenues for the seismic characterisation of thermal regime in disparate settings and varied disciplines.

DECLARATION

University of Manchester PhD by published work Candidate Declaration

Candidate Name: Arka Dyuti Sarkar

Faculty: Science and Engineering

Thesis Title: Reflection Seismic Thermometry

I declare that the thesis has been composed by myself and that the work, other than that identified below, has not be submitted for any other degree or professional qualification. I confirm that the work submitted is my own, except where work which has formed part of jointly authored publications has been included. My contribution and those of the other authors to this work have been explicitly indicated below. I confirm that appropriate credit has been given within this thesis where reference has been made to the work of others.

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THESIS PRESENTATION

This thesis is presented in a paper journal format following the standards given by the University of Manchester. This thesis is entitled “Reflection seismic thermometry”. This thesis comprises seven main chapters with chapters 3 – 6 dedicated as paper publications for technical journals. Chapter 3 is based on the work in the Lüderitz Basin, offshore Namibia and the development of the methodology. Chapter 4 is based on the Blake Ridge, offshore USA and the calibration of the methodology. Chapter 5 is based on the North Viking Graben, North Sea and is both a blind test of the modelling workflow and a ground truthing exercise. Chapter 6 is also based on the North Viking Graben and contrasts the impact of velocity input on the workflow, revisiting the results from Chapter 3 to see how they might change in light of these new findings.

Each chapter is detailed as follows:

Chapter 1 – *Thesis overview*

This chapter introduces the rationale behind the project and gives an overview.

Chapter 2 – *Thermal regime in the context of the subsurface*

This chapter provides context in terms of the subsurface thermal regime, explaining the concepts that underpin the work developed in this thesis. This includes a discussion of the present state of thermal data in the subsurface and leads on to a brief summary of the case study locations covered in this work and the data utilised.

Chapter 3 – *Temperature from seismic reflection*

This chapter contains the first technical paper that is aimed to be published in First Break.

Contribution of co-authors: Prof Mads Huuse (seismic expertise and discussions regarding the development of the workflow along with manuscript review).

Chapter 4 – *Seismic characterisation of thermal regime: a Blake Ridge study*

This chapter contains the second technical paper aiming for publication in Geochemistry, Geophysics, Geosystems.

Contribution of co-authors: Prof Mads Huuse (seismic expertise and discussions regarding the development of the workflow and manuscript review).

Chapter 5 – *Subsurface temperature of the northern North Sea*

This chapter contains the third technical paper aimed to be published in Basin Research.

Contribution of co-authors: Prof Mads Huuse (seismic expertise and discussions regarding the results in context of the calibration data).

Chapter 6 – *Impact of velocity input in seismic thermometry*

This chapter contains the fourth technical paper aiming for publication in Leading Edge.

Contribution of co-authors: Prof Mads Huuse (seismic analysis and discussions regarding manuscript review).

Chapter 7 – *Synthesis*

This chapter summarises the results given by the various studies conducted during this project and how it fits with the proposed aims; how it contributes to existing knowledge in and study of the subsurface thermal domain in general; and potential for future avenues of work.

1. Thesis overview

1.1 Why is subsurface temperature important?

An understanding of the subsurface thermal regime is beneficial to many disciplines including petroleum and geothermal energy extraction, gas storage and sequestration (Ringrose, 2020; Stephenson, 2018). In petroleum exploration temperature is critical for petroleum systems elements such as the degree of transformation of organic matter trapped in source rocks to hydrocarbons (Beardsmore & Cull, 2001); and the type of hydrocarbons and their proportion (Gluyas et al., 2009). The temperatures in the subsurface also help development geologists understand reservoirs better, as temperature conditions can affect porosity for example (Allen & Allen, 2013). As fluid diffusivity varies with temperature, understanding this can maximise recovery (Davarpanah & Mirshekari, 2020; Hognesen et al., 2005). Understanding temperatures currently in the reservoir is also advantageous for the energy transition. Carbon capture and sequestration (CCS) projects could benefit from understanding the temperature regime in order to estimate the total volume of CO₂ that may be stored and where injectivity and diffusivity might be greatest, thus highlighting potential areas of injection points and areas most at risk of leakage (Vilarrasa & Rutqvist, 2017). Geothermal energy prospecting clearly benefits from an enhanced understanding of subsurface temperature distributions when scoping out projects for heat and electricity generation from subsurface heat (Gluyas et al., 2018). The nuclear waste storage sector also benefits from knowledge of subsurface temperature, as temperature can affect the breakdown of the radioactive matter (Christofi & Philip, 1997). Subsurface microorganisms are temperature dependant and have been shown to help in bioremediation of petrochemical pollution (Basso et al., 2005).

1.2 Rationale

The traditional approach for determining subsurface temperature has been for direct measurement, usually through invasive means such as drilling and lowering instrumentation into the resulting borehole (Beardsmore & Cull, 2001) or measuring/estimating heat flow on or near the surface (Grevemeyer & Villinger, 2001; Martin et al., 2004; Pribnow et al., 2000; Serié et al., 2017) or inferring subsurface temperature from trends or analogues with other comparable locations where the geotherm is known (Macgregor, 2020; Minshull, 2011).

The aim of this PhD work is to develop a robust methodology for determining subsurface temperature using a non-invasive remote sensing approach based on reflection seismic data. The approach pursued by this project is a novel method for determining the thermal condition of a sedimentary basin which has been enabled by the advent of workstation computing and high-quality seismic velocity datasets.

In offshore areas, borehole data may be sparse or absent. In contrast, modern 2D & 3D seismic reflection datasets have a far greater likelihood of coverage in such areas, with this coverage being far more laterally and vertically extensive than borehole data. This presents a rich dataset available far in advance of drilling, particularly in frontier basins. The key components of this work are heat flow, acoustic velocity, thermal conductivity and geothermal gradient. Heat flow (Q), thermal conductivity (k) and geothermal gradient (dT/dZ) relate to each other according to Fourier's Law of heat conduction ($Q = k \times \frac{dT}{dZ}$).

Together these three components combine to give an estimate of subsurface temperature based on seismic data input. To do this, acoustic velocity is linked to thermal conductivity through the use of a direct empirical relationship derived from experimental data. Once thermal conductivity is estimated in this manner, by providing constraints on heat flow and thus geothermal gradient, it becomes possible to solve for temperature over the seismic

area/volume. Thus, the project objectives can be defined based on how the understanding of each of these components can be achieved to contribute to the overall thermal picture:

- Use the identification of bottom simulating reflectors (BSRs) at the base of hydrate stability on reflection seismic data to define an isotherm and thus a shallow geothermal gradient – **Papers 1 & 2**
- Continually and iteratively develop an empirical transform between velocity and thermal conductivity for continental margin sediments from existing published experimental data; this will help constrain and define the thermal conductivity of the overburden using seismic velocity data as the input – **Papers 1, 2 & 3**
- Utilise the empirical velocity-thermal conductivity relationship (giving thermal conductivity) with knowledge of the hydrate stability field (giving geothermal gradient) to derive a seismic data underpinned proxy for heat flow (using Fourier’s Law) – **Papers 1 & 2**
- Combine the procedures for use using a common industry software suite (Schlumberger Petrel), to demonstrate accessibility for future use
- Calibrate thermal prediction results against borehole data (where available) to constrain uncertainty and validity – **Papers 2 & 3**
- Test the method in various offshore settings (shallow and deep water) – **Papers 1, 2, 3 & 4**
- Application of temperature prediction methodology in frontier petroleum province, delineating isotherms in the subsurface and implications for prospectivity – **Paper 1**
- Iterative application of workflows to a mature basin with ample borehole control, allowing near-field predictions for mature basin utility such as CCS – **Paper 3**

- Investigate the impact of different types of subsurface velocity data for subsurface temperature prediction – **Paper 4**

1.3 References

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2. Thermal regime of sedimentary basins

2.1 Thermal structure of planet Earth

An understanding of the formation of the Earth is necessary in order to understand the reasons for its present-day thermal structure. This is because the thermal structure of the planet is intrinsically linked to its internal structure and the components that constitute each of the major internal units.

Our solar system was initially a dense cloud of gas and dust (Halliday, 2014). Proto-star formation from the collapse of part of this molecular cloud is believed to have occurred due to its own gravity (Halliday, 2014). As the cloud contracted, it started to rotate with the rotation rate increasing as the cloud became denser. Planetary formation occurred during the T-tauri star phase of the Sun and it happened quickly ($\sim 2 - 5$ My) as the molecular gas cloud condensed into dust (Lissauer, 1993), followed by planetesimals and eventually planets (in a process of collision driven growth) (Wetherill & Stewart, 1993). Modelling has shown that within 10^5 years of the T-tauri stage, planetary accretion was complete (Halliday, 2014). Mercury/Moon sized planetary embryos collided to form Earth-Venus sized terrestrial planets with an enormous amount of energy (in the form of shockwaves and heat) released in such a process, with temperatures exceeding 10000 K (Halliday, 2014). Unlike the gas giants in our solar system, terrestrial planets such as Earth are smaller and accreted from small amounts of silicates and metal phases only, giving them their dense character (White, 2013).

During the planetary accretion stage in the youth of the solar system, the massive amount of energy produced by collisions of planetary embryos would have ensured the planet was mostly in a molten state (Brown & Mussett, 1993). This molten state allowed for the precipitation of heavy/dense material like molten iron to the core while silicates remained in

the outer parts (Fig. 2.1a) (Wood et al., 2010). Molten iron fusing in the core released further heat.

Studies of the Earth's history and its thermal properties have always been linked. Lord Kelvin computed an age estimate (roughly 200 Ma) for the Earth founded on his belief that the Earth was an inert body gradually cooling in space (Beardsmore & Cull, 2001; Halls & Wilkie, 2015). It would take the discovery of radioactivity in 1896 for the realisation that it contributed as a major internal heat source. Thus, the Kelvin age estimate became the minimum age case, only valid for a scenario with zero internal heat production. Essentially the introduction of radioactive heating significantly extended Kelvin's proposed cooling time that underpinned his age estimate for the Earth. The contribution of radioactive heating to surface heat flow is roughly 83% versus 17% from the cooling of the earth (Turcotte, 1980).

Figure 2.1: (a) Scale diagram of the internal structure of the Earth (right) with schematic (left) of the solid outer crust with rheological structuring (that is, asthenosphere and lithosphere); (b) temperature variation within the Earth's interior; (c) Schematic diagram of how mantle convection cells are purported to work within the Earth's interior (displaying the prevailing schools of thought in terms of whole mantle convection and layered convection). Adapted from (Arevalo et al., 2009; Earle, 2019; Panchuk, 2019)

There is no doubt that the Earth's interior is considerably hotter than the surface (Fig. 2.1b). Early models of heat transfer from the deep earth were purely conductive whilst mantle convection (Fig. 2.1c) is now the favoured heat transport mechanism for the bulk earth (Beardsmore & Cull, 2001). Surface heat flow distribution is closely linked to upper mantle temperature (Pollack et al., 1993). Seismic shear wave velocity data supports this (as low shear wave velocities correlate with higher temperatures in the upper mantle).

Conduction remains the dominant heat transfer mechanism in the crust. 40% of outward heat flow originates in the thin outer crust (Beardsmore & Cull, 2001; Hasterok, 2010). Of this, radioactive decay forms the dominant source with frictional heat arising from deformation and heat from exothermic metamorphism and diagenetic processes forming the remaining heat contributors. Heat distribution in the crust is not uniform as radioactive isotopes are found in greater quantity in certain lithologies (Fig. 2.2); heat from friction between plates will only really occur at plate margins; and diagenetic or metamorphic processes only occur at specific geological conditions.

Radioactive heat is from the decay of unstable isotopes. The isotopes of three elements predominantly make up radiogenic heat contribution: uranium (U^{238}), thorium (Th^{232}) and potassium (K^{40}) in that order (of heat production) (Mareschal & Jaupart, 2013). Potassium occurs in clay minerals; rock forming minerals (such as feldspars or mica) and in evaporites (Schön, 2015a). Thorium is associated with acidic and intermediate rocks, whilst uranium is also associated with acid (and intermediate) rocks. Uranium can also be found in phosphates and organic matter and can exist independently (not as a rock forming mineral) making its crustal distribution heterogeneous (Schön, 2015a).

Figure 2.2: Histogram displaying the mean radiogenic heat production of selected igneous and sedimentary rocks. Adapted from (Schön, 2015a).

The greatest heat production is found in acidic rocks (Fig. 2.3). Consequently, oceanic crust with its primarily basic rock contribution has very little contribution from internal heat production to oceanic heat flow (Hasterok et al., 2011; Hasterok, 2010).

Figure 2.3: Links between the radioactive tendencies and rock types from Schön (2015a). The y axis for sedimentary rocks essentially represents an increase in clay content, with the increasing radiogenic heat production coming from the increase in the presence of potassium for example. The y axis for igneous rocks shows the transition from mafic (basic) to felsic (acid) rocks.

Frictional heating from faults tends to occur in those faults where the movement is a continuous creep, with the energy required to overcome friction in this instance being dissipated as heat to the surroundings. In other faults, the sudden burst of energy required to overcome friction is dissipated as the elastic energy that manifests as and causes earthquakes. It has remained difficult however to quantify the exact contribution of friction at fault interfaces to heat generation. Studies done from active margins such as the Cocos subduction zone in Mexico and the Cascadia subduction zone near Vancouver island, have shown that surface heat flow readings did not have a frictional heating component (Beardsmore & Cull, 2001).

Metamorphic reactions, due to their endo- or exothermic nature, also act as heat sources/sinks in the crust. In general, most commonly encountered metamorphic processes are endothermic in nature with dynamic metamorphism being exothermic. Practically,

metamorphic processes act to reduce surface heat flow as there are very few instances where metamorphic processes act as a heat source (Beardsmore & Cull, 2001).

2.1.1 Heat flow in the crust

Generally, in continental settings heat flow or heat flux can be found to be lower in stable settings than in active regions (Fig. 2.4a). When examining crustal thickness (Fig. 2.4b) against continental heat flux, it is seen that there is a negative correlation (Mareschal & Jaupart, 2013). Uranium and thorium, highlighted earlier as two of the three elements most responsible for radiogenic heat generation, tend to become concentrated in the continental crust. This has effects at both global and local scales. At the global scale, the concentration of these elements in the crust depletes the convective mantle as a consequence, leading to impacts on the earth's thermal evolution (Jaupart et al., 2016). At a local scale, this results in continents with their own intrinsic thermal regime.

Figure 2.4: (a) Heat flow variation across continents with stable continental areas having heat flow variation governed primarily by changes in crustal thickness and composition. (b) Crustal thickness variations. From (Mareschal & Jaupart, 2013)

In the oceanic domain, heat flow measurements are found to be greatly impacted by the occurrence of hydrothermal circulation, particularly in young ocean crust (Lister, 1972). Sediment cover exceeding 400 m would be necessary to filter out the impact of the hydrothermal fluid flow disruption on heat flow (Hasterok, 2010). This implies very little of the actual seafloor has sufficient sediment cover to counteract the hydrothermal circulation

effect. Consequently, a systemic low heat flow bias is observed in measurements from shallow sediment highly ventilated by thermal circulation. Proximity to nearby seamounts is also a factor impacting oceanic heat flow. Statistical analysis has found that distances greater than 60 km from the nearest seamount are sufficient to negate the impact of hydrothermal fluid circulation on measurements of oceanic heat flow (Hasterok et al., 2011). Oceanic heat flow is not just impacted by hydrothermal fluid circulation. It is also affected by sedimentation, sediment compaction and thermal rebound. The greater the rate of sedimentation, the more heat flow is depressed, as sediments deposited tend to do so at the bottom water temperature which leads to a depressed thermal gradient. Sedimentation rates of 100 m/m.y. can reduce heat flow 10% though most of the ocean floor does not experience such high sedimentation rate (Hasterok et al., 2011). Only at the mouths of rivers with high sediment discharge, such as in the Bay of Bengal, would the very high sedimentation rates conducive to perceivable heat flow reduction be observed.

2.2 Present state of knowledge

The earliest records for thermal gradient in the earth date back to the 19th century and were compiled incidentally by Fourier (Fourier, 1827). Fourier is important as his name is given to Fourier's Law, the fundamental relationship between heat flow, thermal gradient and thermal conductivity that underpins the work pursued in this project. The law is as follows

$$Q = k \times \frac{dT}{dz} \quad (1)$$

Where Q is heat flow (mWm^{-2}); k is thermal conductivity ($\text{W m}^{-1} \text{K}^{-1}$) and dT/dz is geothermal gradient ($^{\circ}\text{C km}^{-1}$).

Thermal gradient is a vector quantity as it is dependent on temperature distribution in all 3 dimensions. This gives thermal gradient as following:

$$\Delta T = \frac{\delta T}{\delta x} i + \frac{\delta T}{\delta y} j + \frac{\delta T}{\delta z} k \quad (2)$$

Where ΔT is thermal gradient ($^{\circ}\text{C km}^{-1}$); T is temperature ($^{\circ}\text{C}$);

In practice the assumption that is invariably applied is that the maximum thermal gradient in the upper crust is vertical. This gives the one-dimensional approximation for geothermal gradient that is applied in this study.

$$\Delta T = \frac{\delta T}{\delta z} \quad (3)$$

Where ΔT is thermal gradient ($^{\circ}\text{C km}^{-1}$); T is temperature ($^{\circ}\text{C}$); z is the vertical distance (km)

2.2.1 Thermal data measurement in upper crust

Thermal measurements from deep drilling only extend to a maximum depth of roughly 12 km, which is far less than the 6370 km radius of the Earth. Consequently much of the knowledge of the earth's interior is deduced using indirect means, such as seismic methods or gravity data (Beardmore & Cull, 2001). Direct measurement of thermal properties in the crust is therefore limited to relatively shallow depths in the context of average crustal thicknesses.

During petroleum exploration heat generation may be ascertained from well log data, particularly natural gamma ray logs (NGL). These rely on an empirical relationship between gamma ray count and the concentration of radioactive minerals (such as uranium, thorium and potassium), hence the term 'hot shale' (Schön, 2015a).

Deep water probes (Fig. 2.5) usually consist of thermistors placed in the metal lining of a probe designed to penetrate the soft substrate at the seafloor. Once frictional heating from penetration itself has subsided/dissipated the probes can compute thermal gradient across each inbuilt thermistor interval. This is predicated on the probe fully penetrating the substrate though it may get deformed in the process of penetration. These early Bullard-type probes (Fig. 2.5a) were followed by the Ewing-type probes (Fig. 2.5b) that had a hollow shaft allowing for core sample thermal conductivity analysis to happen concurrently to temperature data

collection. Since the 1970s Lister-type probes (Fig. 2.5c) with their distinct violin bow structure (with a sturdy metal strength member and thermistor mounted in a thin sensor tube akin to a bow and string respectively) have been used (Hyndman et al., 1987). Modern data storage and transmission advances have obviated the need for physical recovery of such probes for data retrieval. As with wireline logging today, data storage is held locally on the device with real time data transmission capability.

Figure 2.5: Types of heat flow probe. (a) Bullard type; (b) Ewing type; (c) Lister type. Thermal transistors typically have 25 cm spacing. From (Beardsmore & Cull, 2001).

2.2.2 Heat flow databases

Over time there have been numerous attempts to do a global analysis of heat flow data (Davies, 2013; Hasterok et al., 2011; Hasterok, 2010; Lucazeau, 2019; Pollack et al., 1993). Often such heat flow compilations can have a regional basis, covering whole continents such as Africa (Macgregor, 2020) or North America (Blackwell et al., 1990); or basin wide such as in the North Sea or offshore Congo (Lucazeau et al., 2004; Ritter et al., 2004). From the earliest heat flow records for continents (Bullard, 1939) and oceans (Revelle & Maxwell, 1952) there have been attempts to compile a global repository for heat flow data, maintained by the International Heat Flow Commission (Fig. 2.6a) (Gosnold & Panda, 2002). Till the 1980s these records were well maintained with regular publication of the organised compilations (Pollack et al., 1993) however these efforts became fragmented in the years since (Lucazeau, 2019). Pollack et al.'s (1993) compilation (Fig. 2.6b) contained 24774 observations with later work by Hasterok & Chapman (2008) containing a combination of 35523 terrestrial and 23013 marine measurements respectively (Hasterok et al., 2011). The most recent compilation by Lucazeau (2019; Fig. 2.6c) has nearly 70000 measurements for heat flow, reflecting the increase in data collection over the decades as technology to do so improved in the form of not just the probes that are utilised but also alternatives to directly sampling for heat flow. Such techniques have included the use of seismic indicators such as bottom simulating reflectors (BSRs) to derive heat flow in continental margins (Fig. 2.7) (Calvès et al., 2010; Grevemeyer & Villinger, 2001; Priyanto, 2018; Shankar & Riedel, 2013; Vohat et al., 2003; Yamano et al., 1982); the integration of oil industry data such as geophysical logs for porosity (such as density; sonic and porosity logs) utilised to estimate thermal conductivity (see Section 2.3.4.2 “Alternatives to direct thermal conductivity measurement” for further detail) (Fuchs & Balling, 2016; Fuchs & Förster, 2013; Goutorbe et al., 2011; Houbolt & Wells, 1980). This increase in heat flow data

points has not changed the global average for continental heat flow (67 mW m^{-2}) but recent oceanic measurements have been found to be 17% higher than past averages (92 vs 79 mW m^{-2} respectively). This is likely a reflection of improvements in oceanic heat flow sampling (Lucazeau, 2019).

Figure 2.6: (a) Map showing distribution of heat flow points from the International Heat Flow Commission's database. (b) A 1993 global heat flow map based on the work of Pollack et al. (1993). (c) The most recent global heat flow map based on the preferred prediction by Lucazeau (2019), highlighting the increase in detail over the last 30 years. Major trends such as high heat flow at convergent plate margins or low heat flow in continental settings underpinned by old stable cratons, remain unchanged. Looking at the scale bars it becomes clear that anomalous values at extreme ends of the scale from the older prediction have been rectified. All displays utilise a Mollweide projection. Adapted from (Gosnold & Panda, 2002; Lucazeau, 2019).

Figure 2.7: Example of BSR derived heat flow from the Cascadia margin, offshore Canada (Phrampus et al., 2017).

As is evident from Fig. 2.6a, coverage of the heat flow data points is not uniformly extensive across the globe, with concentration of measurements in areas of greater interest (be it for commercial or academic reasons) such as continental margins or oceanic basins (Uyeda & Horai, 1982). In regions such as Greenland and Antarctica with their extensive glacial and ice cover, sampling is prohibitively difficult and thus there is little to no coverage (Mareschal & Jaupart, 2013). Data coverage globally can be quantified as representing only 2.7% of the Earth's surface if using a $0.5^{\circ} \times 0.5^{\circ}$ grid (Lucazeau, 2019). To account for this there have been attempts to extrapolate (or even predict) through modelling, heat flow across the globe with the most recent work by Davies (Davies & Davies, 2010; Davies, 2013). These predictions primarily depend upon the data points, but predictions are underpinned by variables that might include the geology or the age of the crust in the area of interest. So in an oceanic crustal setting, heat flow is based on crustal thickness in order to mitigate for the impact of measurement perturbation due to fluid flow (Davies, 2013). Should there be a lack of data,

geological models are relied upon using parameters such as the elevation of seafloor for example. However, Jaupart & Mareshchal (2013) pointed out that the relationship between geology and heat flow is too weak to be a suitable proxy. This has led to studies making use of multiple proxies to mitigate for this (Goutorbe et al., 2011). Such proxies include upper mantle shear wave velocities and magnetic field strength. Beyond the spatial bias of scientific investigations favouring high heat flow domains, global estimates such as Davies (2013) (Fig. 2.8) or any spatial grid based study such as that will have implications linked to the grid spacing used. That study used a $2^{\circ} \times 2^{\circ}$ grid which undoubtedly dampens the intrinsic heat flow variability shown to occur at length scales 50 km or lower (Davies, 2013; Goutorbe et al., 2011). Depending on the grid spacing, the interpolation methods used will also have an impact on the statistical reliability of the predicted result, though this is still useful to provide first order estimates in zones that may be entirely lacking in heat flow data.

Figure 2.8: An example of a model driven global heat flow estimation map from (Davies, 2013). The $2^{\circ} \times 2^{\circ}$ equal area grid is distinguishable.

2.3 Approaches to determine thermal structure

Traditional well logging is conducted shortly after drilling with the tool lowered to the bottom and logging being conducted as it is drawn up. Temperature logging however is done in the other direction, so as to reduce the possibility of ambient temperature in the hole being disturbed by the lowering of the tool itself. Also, temperature logging is ideally conducted after allowing sufficient time for temperature in the hole to equilibrate back to ambient temperatures (the very act of drilling and the circulating drilling fluids perturb the downhole temperature conditions). Due to temperature logging running counter to the time and directional standards for regular well logging, many wells lack temperature log data. In onshore boreholes, it may be possible to revisit it for detailed temperature logging after thermal equilibration, but offshore wells are usually abandoned, making revisiting them for temperature logging practically unfeasible.

Often temperature logging is now conducted concurrently as part of commercial wireline logging services, but this naturally suffers from the short interval post drilling not allowing for the borehole to equilibrate to ambient temperature. Bullard (1947) found that it can take between 10 to 20 times the drilling time for the borehole to equilibrate back to ambient temperature. To counteract the thermal disturbance caused by fluids linked to drilling necessitates the use of correction procedures.

Large diameter boreholes, or those that are washed out resulting in wider bore sizes, coupled with a geothermal gradient of $25\text{ }^{\circ}\text{C km}^{-1}$ is sufficient to induce a convection cell. These cells generally do not significantly impact the broader temperature trends, but do reduce the signal to noise ratio of temperature logs (Beardsmore & Cull, 2001).

2.3.1 Bottom Hole Temperatures

Bottom hole temperatures (BHT) constitute a large dataset of temperature available for oil and gas wells. Their importance in the oil industry arises from the manner in which these measurements are taken, and the fact that the highest temperature is always assumed to be at the bottom of a hole. When drilling, it is not a continuous process as interruptions occur for a number of reasons. Usually these involve the changing of a drill bit; running wireline logs; or to case the well. The tool string lowered into the hole has generally contained a temperature sensor and this is what gives the direct temperature measurement of the fluids at the current bottom of the hole. However as alluded to earlier, BHT does not truly reflect the virgin rock temperature (VRT), and this has led to the development of a number of methods to address this disparity. Corrections for this include that developed by Cooper & Jones (1959), and an empirical correction used by the American Association for Petroleum Geologists (AAPG) (Deming, 1989) for example. However, the most widespread BHT correction method in the hydrocarbon industry is the Horner plot method (Cornford, 1998; Horner, 1951; Lachenbruch & Brewer, 1959). The Horner plot was originally developed as a means to predict reservoir pressure recovery. Its basis in temperature correction arises from an observed similarity in the behaviour of in situ temperature and pressure when disturbed by drilling. The Horner correction is governed by three main parameters that are:

1. BHT
2. Time elapsed between cessation of fluid circulation and BHT measurement
3. Time elapsed between cessation of both drilling and that of fluid circulation

The accuracy of the Horner plot correction (Fig. 2.9) is tied to the reliability of the above parameters and their record in documentation. Often these times are rounded off in completion reports, whilst temperatures might not be recorded for large spans between

logging runs with it also being rounded off. These naturally introduce bias to the results and reduce accuracy, the degree to which is hard to precisely quantify. Horner corrections may underrepresent true formation temperature (Deming, 1989).

Figure 2.9: Example Horner plot for BHT correction from Beardsmore & Cull (2001). Here Δt is the time elapsed between cessation of fluid circulation and measurement of T (i.e., BHT); and t_c is the time elapsed between cessation of drilling and cessation of fluid circulation. Time (t_c) usually has units of hours. It is a graphical correction technique whereby true formation temperature may be determined by extrapolating to infinitely long warming times and infinitely short cooling times (Cornford, 1998). VRT is found on the Y-intersection of straight lines through the temperature vs time points for each depth.

2.3.2 ODP thermal measurement tools

Ocean Drilling Program (ODP) borehole data (Fig. 2.10) due to the openly accessible nature can often provide the basis for many types of studies. In this work ODP data have been utilised for chapters 3 & 4 to provide constraints on thermal variables such as thermal conductivity; geothermal gradient and heat flow. Thus, it is important to consider the tools used by the ODP and its successors (IODP) and predecessors (DSDP), in making subsurface measurements, and

the implications these might have on the readings. 'ODP' is used here to refer interchangeably to its current iteration (IODP), to the ODP and to the Deep Sea Drilling Project (DSDP).

Figure 2.10: Combined map of all conducted sites of the various iterations of ocean drilling programmes. (From <https://iodp.tamu.edu/scienceops/maps.html> first accessed August 2016)

2.3.2.1 Thermal conductivity tools

ODP thermal conductivity measurements are made primarily with two tools: the needle probe method (NP) (Von Herzen & Maxwell, 1959) and the quick thermal conductivity meter (QTM) (Hyndman et al., 1987). While the QTM method can be applied to all sediment sample types (soft sediment or lithified) and basement rocks, the NP method is typically preferred for soft sediment samples. This is because it is able to negate the effect of porewater evaporation in soft sediment (Horai, 1982).

For the NP method (Fig. 2.11), sample preparation requires the drilling of a hole or groove of the probe dimensions, into which the latter can be inserted. For lithified sediment where this may prove difficult, split flat surfaces of a sample must suffice. No special contact material is utilised, with water present acting to facilitate heat exchange between the sample and probe. How a needle probe works is through noting the temperature-time response of the core sample to the transient line-source heating up (Pribnow et al., 2000). As the needle probe thermal conductivity value is provided for a plane perpendicular to the needle axis, it is important to note the orientation of needle insertion relative to the sediment bedding direction. This is because any anisotropy parallel to bedding can affect the measurement and lead to bias in the results (Grevemeyer & Villinger, 2001).

Figure 2.11: Needle probe thermal conductivity set up displaying how it may be inserted into the sample (a) and the internals of the probe itself (b). From (Cortes et al., 2009)

Sample preparation for the QTM is not as involved as the probe itself is constituted of a line heat source and temperature sensor mounted in a thermally insulating material having a flat smooth surface. This is directly attached to the sample for measurements to be conducted. Therefore, the quality of results is predicated by the contact between the probe and sample. Weighting the probe in order to ensure uniaxial pressure on the sample has been one method utilised to ensure goodness of contact (Horai, 1982).

2.3.2.2 Temperature measurement tools

Temperature measurements in the borehole are made from a suite of 3 different tools available to the ODP. These include the advanced piston corer (APC) (Fig. 2.12); water sampler temperature probe (WSTP) (Fig. 2.12); and the Davis-Villinger temperature probe (DVTP). The APC tool is embedded in the cutting shoe of the piston corer itself, and thus measures in situ temperatures during regular piston coring operations (Pribnow et al., 2000). Note that the APC tool and its results may be referred to as the ADARA (processing software company) temperature tool within ODP literature. The absolute accuracy is nominally ± 0.1 K with the APC tool (Grevemeyer & Villinger, 2001). Subjective temperature-time curves are used to fit APC probe data to restore to equilibrium temperatures and negate the effect of frictional heating upon insertion of the probe.

APC temperature data is smoother than WSTP data as the data logger is more stable and the tool calculates the reading from an average of four records (Paull et al., 1996). However below certain depths, lithification hinders the penetration of the former (Grevemeyer & Villinger, 2001). This leads to the application of the WSTP probe. It too penetrates sediments ahead of the drill bit in order to counteract the perturbation effect of drilling fluid circulation on the measurements. A hybrid of two earlier tools (Uyeda Temperature Tool & Barnes Fluid

Sampler), it has a resolution of 0.02 K at room temperature with this falling off at increasingly high temperatures (Pribnow et al., 2000). It has an accuracy of ± 0.1 -0.2 K (Paull et al., 1996).

Figure 2.12: Examples of the temperature sampling tools used such as the Adara heat flow probe and the WSTP, adapted from (Pribnow et al., 2000).

The DVTP was designed as the successor to the WSTP and had a probe deliberately designed to be more cylindrical across its entire length in order to more closely approximate a line source. It was developed during ODP Leg 164 over the Blake Ridge and benefits from triple thermistors. This allows it to not only determine thermal gradient, but function over a wider range of temperatures, with one of the thermistors able to be calibrated for operations in high temperature borehole conditions (albeit at the cost of reduced resolution) (Paull et al., 1996). Heat flow is not directly measured by ODP studies, instead it is derived from borehole data using the Bullard Method, eponymously named after the earliest (continental) heat flow measurements by Bullard in South Africa (Bullard, 1939). This method assumes a linear relationship between temperature and the thermal resistance of sediments. The resulting

Bullard plot (Fig. 2.13) is only straight provided conditions are steady state, conductive and lack any internal heat production (Pribnow et al., 2000).

Figure 2.13: Example Bullard Plot shown for ODP Leg 164 Hole 994C (Blake Ridge) (see Chapter 4) from (Pribnow et al., 2000).

2.3.3 Indirect temperature indicators

Direct temperature measurement methods and their tools have been discussed previously. However, there are instances where indirect indicators for temperature may be utilised, which may include the groundwater thermochemistry, Curie depth temperature or gleaning temperature information from mantle xenoliths. Ultimately the aim of this project is to test the efficacy of a seismic derived means for indirect temperature field computation, seismic thermometry if you will, so it is important to place it in context of other such existing methods. In deep geothermal reservoirs, geochemistry may be utilised to determine temperature information. It is underpinned by the temperature dependence of solubility of dissolved solids in groundwater and thus works at high temperatures ($>200\text{ }^{\circ}\text{C}$) (Beardsmore & Cull, 2001). The Curie depth is related to the depth at which the Curie temperature is reached (Blakely, 1988). It is the temperature at which minerals lose their magnetism. As the Curie temperature

for major magnetic rock forming minerals are known, it becomes possible to determine an isotherm. However, the Curie depth can often coincide with a compositional boundary between rocks bearing magnetic minerals (magnetite being the most common) and those lacking it (Rajaram et al., 2009). Correlating with deep sounding seismic or gravity data the Curie temperature isotherm may be identified should it not coincide with a velocity or density boundary (Beardsmore & Cull, 2001; Tewari et al., 2018). The latter boundaries would more likely represent the aforementioned compositional changes rather than a discrete isotherm. As the Curie temperature of magnetite is 580 °C, Curie depth in most continental settings is set as such. Magnetic surveys can thus be utilised to demarcate this deep thermal marker based on the Curie isotherm.

Depth related diagenetic or metamorphic mineral changes may also indirectly provide information regarding temperature. For those studying the deep earth, analysis of mineral assemblages of xenoliths in country rock brought up can be one such indicator (Hasterok, 2010). Similarly the transition from Opal-A to Opal-CT bearing sediments due to changing pressure-temperature conditions at depth, is another such marker for temperature and this is discussed later in Section 2.4.2.

2.3.4 Deriving thermal conductivity

Thermal conductivity is a tensor quantity, not a scalar. This is because it can be anisotropic, varying in different directions through the same medium. By definition thermal conductivity is a measure of how well, not how fast, heat is conducted through a material (Gu et al., 2017). That is, it characterises the heat transfer capability as a result of temperature gradient (Mielke et al., 2017).

To understand thermal conductivity, briefly the heat transfer theory must be discussed (Clauser & Huenges, 2013; Williams & Anderson, 1990). Phonon conduction theory is the

dominant mechanism for heat conduction in the crust (Beardsmore & Cull, 2001). It can be thought of at the molecular level as the propagation of phonons across interatomic bonds. Phonons themselves are a means of representing vibration states (acoustic wave packets) as a particle (Pribnow et al., 1993). This theory allows us to visualise the thermal conduction process but only at the level of individual crystals. To quantify in situ thermal conductivity, cannot rely on phonon conduction alone as the latter is a product of the interaction of all the different mineral components that tend to constitute a rock. Thus, mixing laws are required (Mielke et al., 2017), the three most common ones being:

1. Harmonic mean model (applied for simple horizontal layered strata arranged in the direction perpendicular to heat flow)
2. Arithmetic mean model (applied for geological instances involving vertical contacts such as a vertical dyke and the contact metamorphic zone; faults; etc.; that is, instances where layers are arranged parallel to the direction of heat flow)
3. Geometric/square root mean (applied for a mixture of lithologies).

The geometric mean model is most applicable for the scenarios encountered subsurface (Mielke et al., 2017), especially in a blind setting such as the premise of this work. It is safe to assume that the lithologies encountered will be an assemblage of various minerals.

2.3.4.1 Thermal conductivity measurement

Thermal conductivity measurement methods are either steady state or transient. In the steady state method, a sample of unknown thermal conductivity is compared to a known one. This tends to yield results with more accuracy and also definitively defines thermal conductivity in the desired direction. However, it is only possible in consolidated rocks. In transient techniques the sample is subjected to a heat impulse and the temperature response examined to deduce thermal conductivity. In doing so, thermal conductivity is averaged over two or

three dimensions, thus allowing it to be applied to a broader swathe of samples (crucially including unconsolidated samples).

The most common steady state measurement is using the divided bar apparatus (Fig. 2.14). In this method, the temperature drop across a disc shaped sample of saturated rock is compared to a disc shaped sample of known thermal conductivity (Popov et al., 1999). For transient technique thermal conductivity measurements, the line source needle probe is the most common. The transient technique was designed in response to the need for seafloor measurements whereby a thermal conductivity estimate was combined with temperature data to infer heat flow (Beardsmore & Cull, 2001). It was used extensively for shipboard measurements (Von Herzen & Maxwell, 1959).

Figure 2.14: Examples of how the divided bar apparatus and needle probe apparatus for steady state and transient thermal conductivity measurements work, from (Schön, 2015b).

Optical scanning is the youngest of the thermo-physical measurement techniques, developed by Popov in the 90's and tested using cores from continental deep boreholes, cores from oil & gas exploration wells and mineral samples (Popov et al., 1999). It too is a transient technique like the line source method but has advantages that have led to its popularity in recent years. The contactless nature of its operation makes it a non-destructive technique that can rapidly and directly measure on core samples that need not require special preparation (such as

needing smooth or plane surfaces). It can also help to estimate the thermal anisotropy and inhomogeneity of rocks. While each of the aforementioned methods have their own associated errors, they can be used interchangeably to determine thermal conductivity (Popov et al., 1999).

2.3.4.2 Alternatives to direct thermal conductivity measurement

Most thermal conductivity data comes with caveats. Many available datasets are based on empirical relationships and uncalibrated core measurements (see Section 2.3.2.1 for core measurement tools) (Brigaud & Vasseur, 1989; Esteban et al., 2015; Lucazeau et al., 2004; Mielke et al., 2017). For regional geothermal studies for example, it is very difficult to acquire/estimate thermal conductivity data directly (Gu et al., 2017). Difficulties with thermal conductivity measurement in borehole arise from poor sensor contact with the borehole wall. It is also a time-consuming process (Gegenhuber & Schoen, 2012). Therefore, it becomes attractive to correlate thermal conductivity with other petrophysical properties that are more easily obtained from borehole or field measurements. As such considerable attention has been devoted to determining methods of estimating thermal conductivity from more easily attainable secondary data such as seismic velocity measurements.

The rocks of the subsurface must be viewed as a multi component system whose parts include the minerals, texture (of grains, such as their shape and size), porosity and the fluid content. In an ideal scenario the composite thermal conductivity of this system would be the summation of the individual thermal conductivity contributions of each component part, combined through the use of a suitable mixing law or effective medium model (Duffaut et al., 2018; Hartmann et al., 2005; Schön, 2015b). To do this would require knowledge of the volumetric fraction of each mineral for example, normally ascertained using sufficient logging data (Brigaud et al., 1990). The premise of this work is to present a remote sensing method,

and as such it is not feasible to be able to determine thermal conductivity through the individual components and thus it becomes necessary to pursue a direct, empirical approach. Seismic data underpins the thermometric process developed in this work. While the aim is to derive information about the thermal properties of the subsurface, seismic data intrinsically records the elastic properties of the subsurface (Mavko et al., 2009). Thus, for a direct empirical relationship between a thermal property such as thermal conductivity and an elastic property such as acoustic velocity, it becomes necessary to understand the individual controls on these. The attention to this direct relationship over time has been in the form of extensive experimental studies (see Section 2.3.4.3). These studies have shown that primary controls on thermal conductivity include mineral composition, texture (grain size and shape), porosity and fractures (Fig. 2.15a) (Gegenhuber & Schoen, 2012). Seismic wave velocity is found to be sensitive to these same factors (Fig. 2.15a), providing a basis for a link to be established. Of these primary controls, mineral composition is found to have the dominant contribution on the thermal conductivity. It is generally observed that argillaceous (clay rich) rocks have lower thermal conductivities compared to nonargillaceous (quartz rich) rocks (Mavko et al., 2009). Experimental data shows that for sandstones rich enough in quartz to be considered nearly monomineralic, and with a high degree of cementation, thermal and elastic properties correlate with porosity and saturation in a similar enough manner that direct prediction of thermal properties from elastic properties are valid (Esteban et al., 2015; Pimienta et al., 2018). Porosity is a crucial intermediary. There have been numerous studies examining the link between acoustic velocity and porosity (Fig. 2.15b) (Eberhart-Phillips et al., 1989; Lee, 2003; Mavko et al., 2009; Velde, 1996), and similarly the relationship between porosity and thermal conductivity (Fuchs & Förster, 2013; Jorand et al., 2015). Fractures for example contribute to effective porosity and have been shown to impact P-wave velocities by reducing

them (Fig. 2.15a,d) and a similar impact is noted for thermal conductivity too (Zamora et al., 1993).

Fluids also have an impact on thermal conductivity in the shallow subsurface, especially in the marine domain where it is reasonable to assume that the sediments will be fluid saturated. Dry samples have been shown to have a broader spread of thermal conductivity from experimental data (Hartmann et al., 2005). This is attributable to the ratio between fluid properties and matrix properties being larger for a rock and air system than a rock and water system. Theoretically it may be expected then that frozen hydrate saturated sediments above hydrate stability shall show a smaller spread of thermal conductivity than should be expected in sediment from the free gas zone below. Particularly for dry samples, the contribution to thermal conductivity due to lithological heterogeneities (matrix properties) can be masked by the stronger influence of porosity (Hartmann et al., 2005). In contrast wet samples reflect the impact of both porosity and lithological variations equally.

While velocity and thermal conductivity are shown to be sensitive to similar parameters, there remain some inherent assumptions in such an approach. A concern that may arise is to what degree the variability observed in the velocity signal is solely corresponding with thermal conductivity as we would desire, or is it influenced by an external factor such as fluid overpressure. Broadly pore fluid pressure variations track density variations. To obviate this, one solution would be to restrict the application of such a direct transform to regions of hydrostatic fluid pressure only, however it might be the case that slight overpressure would only correspond to a small increase in velocity response (Lee, 2003). As alluded to earlier, empirical relationships for thermal conductivity respond best in isotropic cases, such as monomineralic lithologies. Thermal conductivity itself though is anisotropic and as such mineral orientation has an impact. Correspondingly clay rich rocks with their platy minerals have poorer correlations for thermal conductivity. The platy nature of clay grains versus

rounded sand grains suggest that for clay compaction, the parallel alignment of these platy minerals will lend itself to greater maximum compaction and thus lower final porosity (Fig. 2.15c) (Velde, 1996). It can be expected then that at deeper levels, maximum compaction of these clay rich lithologies will have accordingly low effective porosity, which in turn should contribute to a stronger correlation with both velocity and thermal conductivity. Since the empirical relationship is designed to be utilised across both shallow and deep depth intervals, it is hoped that the impact of the clay lithology variability at shallow depths becomes negated at deeper levels. Ultimately even the best thermal conductivity models are subject to caveats, be it the form of assumptions or specific circumstances where direct relationships might not be as strong.

Figure 2.15: Elastic and thermal properties related against each other. (a) Example of the relationship between thermal conductivity with properties such as density and velocity for igneous rocks from (Schön, 2015b). (b) How velocity varies with both porosity and differential pressure (Lee, 2003). Taken from experimental data for overpressured and unconsolidated sediments offshore (where BGTL is Biot-Gassmann theory by Lee). (c) Variation of porosity with depth (Velde, 1996), showing how there is an apparent 500 m threshold beyond which a log relationship becomes necessary. (d) Experimental data highlighting the link between thermal conductivity and porosity (Mielke et al., 2017). (e) Thermal conductivity variation with mineral content, in this case the proportion of clay minerals (Brigaud & Vasseur, 1989).

2.3.4.3 Thermal conductivity derivation from physical measurements

Numerous correlation studies have been conducted to derive thermal conductivity from physical properties (some examples in Fig. 2.16) (Griffiths et al., 1992; Gunn et al., 2005; Hartmann et al., 2005; Kukkonen & Peltoniemi, 1998; Popov et al., 2003; Rybach & Bunterbarth, 1982; Zamora et al., 1993). Many previous studies have sought to correlate thermal conductivity to other petrophysical properties using regression analysis. The Griffiths et al. (1992) study correlated thermal conductivity and wireline log porosity. It used a very wide range of rock types which is preferable and concluded that the greater range of rock type samples taken will increase the robustness of the study. A linear regression was used for each lithology. The Zamora et al. (1993) study tested existing empirical relationships between thermal conductivity and velocity on samples of a near isotropic quartz rich sandstone sampled at varying porosity. Direct measurements were made on the samples. It found a linear correlation for wet samples. The Kukkonen & Peltoniemi (1998) study linked thermal conductivity to compressional wave velocity using core samples from Finland. Samples covered igneous, metamorphic and sedimentary rock types. However, the authors found no trend in the results. The Hartmann et al. (2005) study looked at borehole samples drilled into Tertiary Flysch sediments and sought to use regression analysis for the relation between thermal conductivity and seismic velocity, density, etc. concluding that correlations were dependent on local conditions, specifically the type of rock diagenesis (Gegenhuber & Schoen, 2012; Hartmann et al., 2005). This study however did find that a predictive methodology for thermal conductivity is valid and useful even for old and incomplete logging data (when using the appropriate mixing law). This is an important consideration given that many wells were drilled before the advent of modern logging tool suites.

The Gegenhuber & Schoen (2012) study used two separate models instead (a defect model and an inclusion model) of a regression analysis. Their sample set included clastic sediments, magmatic & metamorphic rocks. The inclusion model consists of a homogeneous matrix material with isolated cracks modelled as ellipsoids of differing aspect ratio. The ellipsoidal cracks provide the porosity. Varying the size, aspect ratio and concentration of these ellipsoids changes the porosity. Matrix properties can be altered by changing the mineral composition. The defect model characterises a defect (such as a fracture or crack) parameter based on its relative length. There is good correlation (correlation coefficient 0.74 – 0.9) between thermal conductivity and compressional wave velocity as given by the inclusions model, especially for sedimentary rocks and igneous samples having high quartz ratio. It is seen however that low quartz content samples show a poorer correlation coefficient (0.63) (Gegenhuber & Schoen, 2012). It must be noted that quartz content has a strong positive correlation with thermal conductivity. High quartz content raises the thermal conductivity.

Figure 2.16: Examples from the literature of experimentally measured velocities (V_p) and thermal conductivities (k or λ) directly compared. (a) From (Zamora et al., 1993); (b) From (Duffaut et al., 2018) with the colour bar representing increasing clay fraction; (c) From (Gu et al., 2017); (d) From (Mielke et al., 2017).

Laboratory based studies of thermal conductivities of different lithologies have also been conducted from the viewpoint of building stone analysis (Boulanouar et al., 2013; Özkahraman et al., 2004). This is because natural building stone of low conductivity is attractive as thermal insulation for construction. These studies found directly proportional relationships between P-wave velocity and thermal conductivity, though it must be noted that lithologies were limited to typical building stones such as limestones.

Thermal conductivity models are rare in the literature. Those that do occur are beset by a requirement for a large amount of parameters or are semi-empirical in nature (Esteban et al.,

2015). This limits the applicability of the models in different end use scenarios. PSED (Pimienta-Sarout-Esteban-Delle Piane) model for thermal conductivity only requires two input parameters to predict (Esteban et al., 2015). These are porosity and P wave velocity, both of which can be estimated from wireline logs or directly measured on core samples. However, the underlying assumption is that the sample is entirely monomineralic and clean, which is unlikely to be the case in reality.

2.4 Shallow geothermal gradient using gas hydrate stability conditions

This section will give a brief overview of gas hydrates and the bottom simulating reflectors (BSRs) that they can often cause as they are used to inform the estimation of an isotherm related to the hydrate stability. This in turn helps as a seismic data based proxy to determine not only shallow geothermal gradient (till the base of the hydrate stability zone) but also surface heat flow. These are critical components that form part of the modelling workflow in the Lüderitz Basin and Blake Ridge studies.

2.4.1 Gas hydrates

Schicks (2018) succinctly summarises gas hydrates as “ice-like, nonstoichiometric, crystalline solids composed of a three- dimensional network of hydrogen-bonded water molecules enclosing gas molecules in defined cavities of different sizes”. Methane hydrate is the most abundant gas hydrate found globally, with it constituting nearly 99% of hydrocarbon molecule trapped in naturally occurring hydrates with only minor quantities of CO₂ or H₂S being present (Beauchamp, 2004; Collett et al., 2009). As such the term methane hydrate is often interchangeably used to mean gas hydrate. In the hydrocarbon exploration industry, gas hydrates are of note for their impact as a subsurface drilling hazard and for affecting oil and gas infrastructure such as pipelines onshore (Boswell et al., 2012; Gao, 2008; Swart, 2009).

Hydrate studies are of importance in other disciplines too such as measuring their contribution and impact on climate as a major methane sink; as well as their influence on slope instability and submarine sediment remobilisation through hydrate dissociation (Gabitto & Tsouris, 2010; Kretschmer et al., 2015). Proposals also exist to explore the resource and exploitation potential of hydrates as an energy resource for nations typically lacking in endemic hydrocarbon resources of their own (Collett, 2002; Shankar & Riedel, 2013).

Figure 2.17: The white material pictured formed under the mussel encrusted carbonate rock is gas hydrate as pictured in the Gulf of Mexico. From (Ruppel & Kessler, 2017)

2.4.1.1 Distribution & quantification

Naturally occurring gas hydrates can be found onshore in high latitude permafrost settings, and in the offshore domain, can be found along both active and passive continental margin settings (see Fig. 2.18) (Collett, 2002; Kvenvolden & Lorenson, 2001; Max & Dillon, 1999; Minshull et al., 2019). Following their discovery in Siberian permafrost (Makogon, 2010), hydrate research has been conducted extensively at the Mallik permafrost research facility (Guerin & Goldberg, 2002; Lee et al., 2009; Uchida et al., 2009). In the oceanic domain, continental slopes and the outer rises of such margins contain gas hydrates, with their

occurrence at depths below 300 m, as this is when the conditions for hydrate stability are met (Kvenvolden & Lorenson, 2001). Low temperatures and intermediate pressures are conducive to hydrate presence as will be discussed in the stability section (Section: 2.4.1.3) and as such permafrost settings and continental slopes satisfy this requirement (Ruppel & Kessler, 2017). Similarly, the lower limit for hydrate occurrence offshore can be determined, with it occurring in reality to 1000 m below the continental surface or ocean floor ("Nat. Gas Hydrates Occur. Distrib. Detect.," 2001).

Figure 2.18: Global distribution of gas hydrates from (Ruppel & Kessler, 2017). Blue circles represent areas with known hydrate (recovered samples), with red circled locations representing areas of inferred hydrate presence (using well logs or geophysical markers such as BSRs). The thickness of the gas hydrate stability zone (GHSZ) shown is theoretical and based on the work of (Kretschmer et al., 2015). Boxed areas represent locations with methane seepage in the upper continental slope linked to hydrate dissociation.

Various authors have attempted to quantify total global hydrate volumes, but with difficulties in direct sampling and the fact that within the zone of hydrate stability in sediments it does not necessarily homogeneously occupy all the pore space, these estimates vary greatly by orders of magnitude (see Fig. 2.19). More specifically, given methane as a greenhouse gas is nearly 84 times more potent than carbon dioxide (IPCC Working Group 1 et al., 2014) it is

quantifying the methane trapped in gas hydrates globally that is of particular interest. As such one estimate based on a review of existing assessments of hydrate volumes estimates 3×10^{15} m³ of methane in place (calculated at standard temperature and pressure (STP)) in global gas hydrates (Boswell & Collett, 2011). Not all clathrate cages contain guest gas molecules, thus less gas can be expected in naturally occurring gas hydrates, which introduces uncertainty in such a quantification (Kastner, 2001). Not all clathrate cages contain guest gas molecules, thus less gas can be expected in naturally occurring gas hydrates, which introduces uncertainty in such a quantification (Kastner, 2001).

Figure 2.19: Cross plot of global estimates of gas in place for gas hydrates against the publication date for the estimate taken from Boswell & Collett (2011). This helps visualise the variability in estimates produced over the decades for global methane hydrate volumes.

2.4.1.2 Structure and formation

Gas hydrates have a cubic crystallographic structure formed when water in the subsurface freezes (Sloan, 1990; Sloan et al., 1998). The structural styles for these hydrate lattice structures have been classified with the cubic structural types 1 & 2 (Fig 2.20a,b) discovered

and described earliest in the literature (Barrer & Ruzicka, 1957; v. Stackelberg & Müller, 1954). The hexagonal structure H (Fig. 2.20c) hydrate was discovered 35 years later, initially only synthesised in the laboratory (Ripmeester et al., 1987). It was later proven that structure H gas hydrate could occur naturally with discoveries made in the Gulf of Mexico (Sassen & MacDonald, 1994). The hydrate structure will influence the nature of trapped gas due to the size of the clathrate cage that it forms (Kvenvolden, 1995). Structure 1 hydrate is most commonly occurring and has the smallest cage structure with typical trapped gas molecules including short chain organic hydrocarbons up to ethanes, while structure 2 hydrates with their larger cage size can accommodate lighter hydrocarbons up to butanes (Kastner, 2001; Sassen et al., 2001). Structure 1 hydrate is most commonly occurring and has the smallest cage structure with typical trapped gas molecules including short chain organic hydrocarbons up to ethanes, while structure 2 hydrates with their larger cage size can accommodate lighter hydrocarbons up to butanes (Kastner, 2001; Sassen et al., 2001). Structure H is able to accommodate larger guest molecules with the largest cavity size (Schicks, 2018; Sloan & Koh, 2007). Cavity number varies per unit cell for different gas hydrate structures, and it must be noted that not all cavities are occupied by guest gas molecules at all times (Ripmeester et al., 1987; Sloan et al., 1998).

Figure 2.20: Examples of a molecular gas hydrate lattice, showing (a) Structure 1; (b) Structure 2; and (c) Structure H gas hydrate crystallography. Adapted from (Schicks, 2018). Hydrate formation is broken down into a two-stage process with hydrate nucleation followed by continuous growth. At the nucleation stage molecules cluster together to form hydrate nuclei, which upon reaching a critical size, transition into a continuous hydrate growth process (Schicks, 2018). Some work has shown that a higher proportion of fine grain content can be more conducive to gas hydrate formation than sands of coarser grain sizes (Heeschen et al., 2016). Nucleation points alone do not facilitate the formation of gas hydrates, it is necessary for there to be an ample supply of both water and gas (in most cases methane). The presence of methane must be in excess of its solubility in pore water for it to become trapped within the clathrate cages (Ruppel, 2011). From a kinematic standpoint, methane hydrate formation is preferred in comparison to a mixed hydrate comprising additional gases. The presence of

sufficient fluid and gas provide the constituent components towards gas hydrate formation, but the conditions for their formation are defined by their stability field.

2.4.1.3 Hydrate stability field

Hydrates are inherently unstable due to the presence of the large cavity discussed earlier at the core of their structure and tend towards dissociation (Beauchamp, 2004). It is only when the cavity is occupied by one or more molecules of a trapped gas that the clathrate structure becomes stabilised. Hydrogen bonding stabilises the lattice structure (Kvenvolden, 1995). It is in this context it becomes necessary to understand the factors governing the stability of frozen gas hydrates, which are primarily impacted by pressure and temperature conditions. The hydrate stability field is a critical part of the temperature estimation workflow presented in this thesis. It underpins the estimation of shallow thermal regime due to the sensitivity of hydrates to pressure and temperature conditions. Most theoretical models on gas hydrate stability are derived from van der Waals's thermodynamic theory. But over time, experimental studies have sought to empirically define the phase relationship for hydrate stability (see Fig. 2.21) in accordance to factors such as pressure; temperature; gas composition; fluid salinity and pore size (Burwicz & Rüpke, 2019; Chand et al., 2008; Dickens & Quinby-Hunt, 1994; Egeberg & Dickens, 1999; Lu & Sultan, 2008b; Tishchenko et al., 2005). These empirical expressions for hydrate stability allow for the determination of temperature and pressure conditions along the phase boundary. If the hydrate phase is known, that is, the gas composition, the fluid salinity and any known impurities, then the phase boundary can be modelled (Fig. 2.22). The intersection between the geothermal gradient and the phase boundary (Fig. 2.22b) should theoretically coincide with the base of the gas hydrate stability zone, which tends to be regarded as the location for a bottom simulating reflector. Therefore, the latter represents an isotherm. It must be noted that gas hydrate stability calculations have

been made with an implicit assumption of a hydrostatic pressure condition due to the shallow seafloor sediments likely be highly saturated (Ruppel & Kessler, 2017).

Figure 2.21: An example of previously modelled hydrate stability curves for a pure methane, salt water phase (salinity 33 g kg^{-1}) and the relation with both experimental and predicted data (Dickens & Quinby-Hunt, 1994; Jager & Sloan, 2001; Lu & Sultan, 2008a; Maekawa, 2001; Sloan et al., 1998).

Figure 2.22: Hydrate stability field diagram for (a) permafrost and (b) marine settings from (Ruppel & Kessler, 2017).

Hydrate phase stability field is linked to its composition, with hydrates comprising gases other than methane having their stability field shifted to higher pressures and lower temperatures (Fig. 2.23) (Jhaveri & Robinson, 1965). The addition of simple salts to the pore fluids has a demonstrable effect of increasing hydrate instability and as such, for the same pressure, the dissociation temperature is lower for salt water systems in comparison to pure water (Dickens & Quinby-Hunt, 1994).

Figure 2.23: Pressure-temperature diagram based on experimental data highlighting how the differing gas composition can affect the hydrate stability field. From (Schicks, 2018).

2.4.1.4 Methane sourcing and environmental implications

As methane is the most commonly trapped gas in frozen hydrates, diagnostic criteria for establishing the source of the trapped gas relies on molecular and isotopic characteristics (see Fig. 2.24) (Bernard et al., 1976). Carbon isotopic analysis indicates microbial methane origin for methane on basis of carbon composition lighter than -60‰ relative to PeeDee Belemnite standard. This is likely derived from the breakdown of organic matter through methanogenic processes in the shallow sediments (Egeberg & Dickens, 1999; Gabitto & Tsouris, 2010; Schicks, 2018). Carbon isotopic compositions above -50‰ from hydrates are indicative of a thermogenic gas origin and correspondingly find trapped gases to be higher hydrocarbons such as ethane or propane (Bernard et al., 1976). Such gases are also derived from organic matter, broken down at depths greater than 1000 m. Biogenic methane can be expected to originate from nearby the hydrate sample location, unlike thermogenic methane which must

migrate long distances from sediment at depth to eventually become trapped in near surface hydrate bearing sediment (Sassen et al., 2001; Tanaka & Clennell, 2003).

Figure 2.24: Compositional fields for biogenic and thermogenic methane using carbon isotopic signature and hydrocarbon gas ratio (R), from a representative global distribution of samples (Bernard et al., 1976; Kvenvolden, 1995).

Gas hydrates also contribute to fluid flow features observable on the seafloor. The seepage of dissociated or free gas from below the hydrate can manifest at the seafloor in the form of venting point pockmarks (Ketzer et al., 2019; Le et al., 2015; Serié et al., 2017). Mound like structures on the seafloor (pingoes) associated with the formation and dissociation of gas hydrate have been noted (see Fig 2.25a) (Serié et al., 2012). The release of methane may even occur violently, showing as mud volcanoes as well as pockmarks linked to brecciated sediments and ejecta (Beauchamp, 2004).

Figure 2.25: (a) High resolution shaded relief of seabed from the Kwanza Basin, offshore Angola highlighting the pockmarks and mounded structures associated with gas hydrate and related fluid flow effects with (b) seafloor bathymetry inset. From Serié et al. (2012).

Warming will have an impact though to differing temporal scales for onshore and offshore hydrates. The deeply buried permafrost hosted hydrates are less susceptible to surficial conditions. Warming of ocean waters will impact the shallow subsurface sediments hosting gas hydrates, altering the conditions for hydrate stability. This can cause increased submarine slope failures. Examples of numerous submarine slump scars in the vicinity of the Blake Ridge indicate the marine slumping in the past may have been instigated by the dissociation of gas hydrates (Dillon et al., 2013). This in turn has been related to the clathrate gun hypothesis, which was proposed as a mechanism for linking late Quaternary interstadials (temporary warming episodes within glacial periods) to carbon isotopic evidence for contemporaneous repeated hydrate dissociation events (Ruppel & Kessler, 2017). This is due to the warming episodes causing warmer intermediate ocean water which leads to dissociation of continental slope hydrates. The methane release from such events would thus be sudden enough for it to not become dissipated through absorption into any sinks, thus being recorded in the isotopic record. The triggering of submarine slumping by hydrate dissociation could disrupt man made undersea infrastructure such as pipelines or undersea data cables (Lemon, 2012). The greater risk might come though from the dissociated free gas volumes below the gas hydrate stability zone (GHSZ) and the potential for its release into the atmosphere.

2.4.1.5 Impact on sediments

Recovered hydrate samples from sedimentary sections have been at the cm scale (Paull & Ussler, 2001). Recovered hydrate samples have been described as having forms that are either cemented; nodular; or occurring as laminae or veins (Collett, 2001). The area extent of the gas hydrate occurrence; reservoir thickness; reservoir porosity and the degree of gas hydrate saturation are all factors impacting the amount of gas hydrates recovered.

A study has shown that hydrate saturation of even 3% is sufficient to positively impact sediment stability (Bernabé et al., 1992). As gas hydrates tend to be hosted in sediments, it is important to note the impact of their presence on the physical properties of the sediment and the microscopic factors that govern these. In one model, gas hydrates are found to envelop sediment grains (Fig. 2.26b), serving as a cement in the process and increasing the sediment thickness (Guerin et al., 1999). In a micromechanical model, hydrate exists purely in the bulk pore spaces and does not contribute to any increase in sediment rigidity (Ecker et al., 1996). Experimental work has demonstrated that even small quantities of hydrate acting as an intergranular cement can serve to increase sediment stiffness (Helgerud et al., 1999). Amplitude variation versus offset (AVO) analysis of the Blake Ridge gas hydrate province seems to suggest that only a micromechanical model can qualitatively reproduce the seismic response (bottom simulating reflector, see 2.4.2) (Ecker et al., 1996; M W Lee et al., 1996).

Figure 2.26: Hydrate cement configurations from (Guerin et al., 1999). Hydrate either is only at the grain contacts (a) or it fully envelopes each sediment grain (b).

Bulk rock physical properties in marine sediment are strongly affected by the presence of frozen hydrate in pore spaces. For example, gas hydrate bearing sediment is characterised by high electrical resistivity (Fig. 2.27b) due to hydrate reducing the effective porosity and electrical conductivity (Hyndman et al., 2001). Resistivity logs, thus prove to be an excellent tool to characterise the in situ properties of gas bearing sediment, including estimating hydrate saturation (Shankar & Riedel, 2013). Hydrate detection is also possible from the perturbation caused in the chloride ion signature in pore water below the hydrate stability zone (Fig. 2.27a) (Ussler & Paull, 2001).

Figure 2.27: Hydrate detection from physical logs taken from ODP Leg 164 in the Blake Ridge (C. K. Paull, Matsumoto, & Wallace, 1996). (a) Negative chloride ion excursions from pore water sampling used to demarcate hydrates. (b) Hydrate zone as recorded by electrical resistivity. From (Collett et al., 2009)

2.4.2 Bottom simulating reflectors (BSRs)

A bottom simulating reflector (BSR) (Fig. 2.28) is traditionally categorised as a continuous and coherent seismic event, that cross cuts the primary sedimentary fabric, whilst mimicking the morphology of the seabed (Berndt et al., 2004; Le et al., 2015; Mackay, 1994). A BSR appears due to an acoustic impedance contrast that can either be caused by the transition from frozen gas hydrate bearing sediment to free gas below, or it can be caused by a diagenetic boundary (Kvenvolden & Barnard, 1982; Yamano et al., 1982). This diagenetic boundary is a lithological

transition from Opal-A to Opal-CT in siliceous sediments at fixed subsurface depths. Sediment that is rich in diatomites gets heated on burial, causing the opal to dissolve and reprecipitate, producing a crystalline fabric and fluid loss (Berndt et al., 2004). As such a diagenetic BSR demarcates an increase in sediment density with depth which results in an increase in acoustic impedance across this boundary. Thus, diagenetic BSRs have the same reflection polarity as the seabed. It is also worth noting that diagenetic BSRs can be mistaken on seismic for flat spots.

Figure 2.28: Single channel seismic image from the Bering Sea highlighting both a hydrate related BSR with its opposite polarity to seabed and a silica BSR with polarity similar to seabed. From (Barth et al., 2009).

Historically, BSRs have been associated with gas hydrates with the earliest studies occurring in the Blake Ridge (Bryan, 1974). Over time this interpretation was extended over continental shelves worldwide (Shipley & Houston, 1979; Stoll & Bryan, 1979). It came to be that the occurrence of a BSR was often considered synonymous with the presence of frozen gas hydrate (Shipley & Houston, 1979), more particularly the demarcation of the base of the gas

hydrate stability zone (GHSZ), though this is not always the case (Holbrook, 2001; Paganoni et al., 2016). In the Blake Ridge for example hydrate presence did not correspond to an observable BSR at Site 994 (Wood & Ruppel, 2000). A gas hydrate BSR is identifiable due to having reverse reflection polarity to the seabed (see Fig. 2.29), due to the drop in acoustic impedance as the transition is made between frozen hydrate bearing sediment within the hydrate stability zone into the sediment bearing dissociated free gas below, that is, free gas zone (FGZ).

Figure 2.29: Schematic illustration of submarine gas hydrate bearing sediment with a free gas zone below the BSR. The BSR marks the base of the GHSZ. It is possible to see the seismic response transitioning from hydrate bearing sediment into the free gas zone FGZ in terms of the decrease in p-wave velocity at the interface. Example taken from a site in Svalbard. From (Haacke et al., 2007).

It is less common that a BSR fulfils all of the criteria (continuous; coherent; cross cutting; mimicking seabed) when viewed on seismic reflection data. For the purposes of this study, guidance on the morphological classification and descriptions of BSRs follow Shedd et al.

(2012). This study examined numerous BSR occurrences in the Gulf of Mexico and categorised these on the basis of morphology (Fig. 2.30b). The traditional view of a BSR has been revised as having a 'continuous' morphology. Instead the most common manifestation is as a 'discontinuous BSR', which is observable as several widely spaced seismic reflectors that generally conform to seafloor bathymetry. Discontinuous BSRs with high observed amplitude are most likely observed at convergent margins, whereas rifted and sheared margins demonstrate BSRs that are continuous in nature, cover a large areal extent and are less distinctive on seismic due to lower amplitudes (Kretschmer et al., 2015). The final category of BSR is the 'pluming' type. A pluming BSR does not follow seafloor bathymetry but instead bulges toward the seabed. These are believed to be caused by areas of high and localised heat flux, due to strong vertical fluid flux, affecting the base of hydrate stability (Shedd et al., 2012).

Figure 2.30: Idealised BSR morphology end members demonstrated on seismic data taken from a representative study in the Gulf of Mexico (Shedd et al., 2012).

2.5 Utilised dataset

The studies conducted have primarily been underpinned by seismic data calibrated by available borehole data. The sourcing of this data has been either through privileged data access from industry sources (hydrocarbon exploration companies; seismic services operators) or from open source datasets hosted as part of internationally funded research endeavours (example IODP). The data used are summarised in Table 1.

2.5.1 Case studies conducted

The case studies have focused on three offshore settings. The order in which they have been conducted is a consequence of the data access and not a deliberate effort to be synchronous with the various stages of development of the methodology. As such the Namibian case study was likely not the ideal setting to develop a new methodology due to the lack of well calibration, instead it serves as an excellent example for applicability to a frontier basin of current interest to the hydrocarbon industry. The main case studies are shown in Fig. 2.31 below. The case studies can be summarised as follows:

1. Lüderitz Basin, Namibia – frontier unexplored deep-water basin with excellent reflection seismic data highlighting the presence of a BSR. Though lacking well control, thermal modelling here can help resolve questions regarding the Aptian source rock interval, a key uncertainty for petroleum systems prospectivity here. Used to develop initial ideas and test the methodology. *Serves as basis for Paper 1/Chapter 3.*
2. Blake Ridge, USA – extensively studied deep-water gas hydrate province. International studies (IODP/ODP) over the past have built up a detailed understanding of the gas hydrate system with abundant well control in the form of open source ODP boreholes and open source seismic reflection data. However, relied on borehole velocities here for thermal modelling. Served as a calibration location for the workflow as well as

demonstrating the applicability using alternate velocity data. *Serves as basis for Paper 2/Chapter 4.*

3. North Viking Graben, North Sea – mature, highly drilled petroleum province having abundant well control with crucial BHT information. Though lacking evidence of gas hydrates unlike previous settings, served as a ground truthing for the workflow using the very recent high-resolution reprocessed reflection seismic and detailed velocity modelling data. Data access to this was last to be granted. *Serves as basis for Papers 3 & 4/Chapters 5 & 6 respectively.*

Figure 2.31: Case study locations for this thesis in the order they were conducted. (1) Lüderitz Basin, offshore Namibia; (2) Blake Ridge, offshore USA; (3) North Viking Graben, North Sea. Bathymetry from (*"The GEBCO_2019 Grid - a continuous terrain model of the global oceans and land,"* 2019).

2.5.2 Data summary table

Table 2.1: Summary of data available for each of the three main case studies covered in chapters 3 – 6.

Case study	1. Lüderitz Basin	2. Blake Ridge	3. North Viking Graben
Geological setting	Volcanic passive margin	Passive margin	Failed rift
Bathymetric setting	Deep water	Deep water	Shallow water
Water depths (m below MSL)	~350-2000	~2600-4000	~75-530
2D/3D seismic reflection volume	Yes	Yes	Yes
Seismic data source	2D - Spectrum; 3D - Serica	3D - OpendTect; NSF	3D - CGG
2D seismic reflection data	Yes	Yes	No
Number of 2D lines	4	1	N/A
2D lines cumulative length (km)	752	19.6	N/A
2D seismic processing	PSTM & PSDM	N/A	N/A
3D seismic reflection data	Yes	Yes	Yes
3D seismic coverage (km²)	4150	349	35410
3D seismic processing	PreSTM	PSTM	PSTM & PSDM
Velocity data type	Seismic processing velocity	Vertical Seismic Profile	FWI and RMO velocities
BSR (gas hydrate polarity)	Yes	Yes	No
Proven gas hydrates	Likely	Yes	N/A
Well control (BHT)	No	Yes	Yes
Calibration borehole count	2	3	139
Borehole data source	1 - ODP; 1 - Norsk Hydro	3 - ODP	139 - NPD
Thermal model area (km²)	4150	349	12042
Petroleum province	Frontier	N/A	Mature

2.6 References

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3. Temperature from Seismic Reflection

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3.1 Abstract

Accurate estimations of present-day subsurface temperatures are of critical importance to the energy industry, in particular with regards to geothermal energy and petroleum exploration. This paper uses seismic reflection observations of bottom-simulating reflections and subsurface velocities coupled with an empirical velocity to thermal conductivity transform to estimate subsurface temperature. The case study is a frontier passive margin extending from the shelf edge to deep water in the central Lüderitz Basin, offshore Namibia. The bottom simulating reflector is used to derive surface heat flow. The thermal conductivity model was applied to seismic processing velocities to determine the subsurface thermal conductivity. Knowledge of surface heat flow and thermal conductivity structure allowed us to estimate subsurface temperatures across the study area. The results suggest the Lüderitz Basin has a working hydrocarbon system with the inferred Aptian Kudu source interval within the gas generation window.

Acronyms

- AI – Acoustic Impedance
- BHT – Bottom Hole Temperature

- BSR – Bottom Simulating Reflector
- BWT – Bottom Water Temperature
- CMP – Common Mid Point
- COB – Continent Ocean Boundary
- FGZ – Free Gas Zone
- GHSZ – Gas Hydrate Stability Zone
- MTD – Mass Transport Deposit
- NOAA – National Oceanic and Atmospheric Administration
- ODP – Ocean Drilling Program
- RMS – Root Mean Squared
- SDR – Seaward Dipping Reflector
- TWT – Two Way Travel Time
- WOA – World Ocean Atlas

3.2 Introduction

Subsurface temperature is a key parameter in subsurface energy extraction from petroleum- and geothermal systems (Bonté et al., 2012; Harper, 1971; Hunt, 1984; Thompson, 1979). Accurate estimations of present-day subsurface temperatures are thus of critical importance to the energy industry. In frontier areas, petroleum source rock maturity is a key uncertainty and without access to bottom hole temperature readings from boreholes, source rock characterisation is reliant on estimation and extrapolation. A crucial component of understanding the subsurface temperature field is how heat is transferred (i.e. heat flow and thermal conductivity) (Sclater et al., 1980). Often there is limited understanding of the variation in thermal conductivity both vertically and laterally in the subsurface domain due to

the difficulty collecting such data. Prior to entry into frontier basins, it is advantageous to determine the source rock deliverability in the area. This is primarily controlled by two factors namely source rock type and temperature history. Along many passive margins the source rocks are at maximum burial depth and thus maximum temperature at the present day. Present day subsurface temperatures are typically acquired from temperature probe measurements that have been acquired through borehole drilling (Fuchs & Balling, 2016). To estimate heat flow and temperature information in adjacent areas often involves the deployment of multiple seafloor probes prior to the drilling stage (Davis et al., 2003). This then requires the extrapolation of data from nearby boreholes using structural and stratigraphic models (Davies & Davies, 2010). This methodology underutilises the available seismic datasets that are often acquired during the early stages of exploration in frontier basins. This paper presents a workflow for using seismic reflection data to estimate subsurface temperature before drilling and applies this to a frontier exploration setting.

It has been shown that gas hydrate identification on seismic reflection data through detection of bottom simulating reflectors (BSRs) at the base of gas hydrate stability zone (GHSZ), can be used for geothermal gradient estimation (Calvès et al., 2010; Hodgson et al., 2014; Serié et al., 2017; Yamano et al., 1982).

This study demonstrates a new workflow for the prediction of subsurface temperatures in frontier basins by first estimating surface heat flow from BSRs and then utilizing seismic processing velocities and empirical datasets relating acoustic velocity and thermal conductivity which allows the estimation of subsurface temperatures throughout the seismic volume.

Figure 3.1: (a) Location map displaying area of interest. (b) Key geological, structural and bathymetric features offshore Namibia are highlighted (contour intervals 500 m), adapted from (Becker et al., 2009; Bray et al., 1998; Gladchenko et al., 1998). (c) Inset map displaying extent of seismic data available, mapped BSRs and transects along which modelling has been conducted.

3.2.1 Geological setting

The study area (Fig 3.1) is in the Lüderitz Basin offshore Namibia, bounded by the Orange Basin to the south, and the Walvis Basin to the north. It is part of the southern West African continental margin. Successive rifting events from the Carboniferous onwards preceded the Mesozoic opening of the South Atlantic, and the breakup of Gondwana (Bagguley & Prosser, 1999; Karner & Driscoll, 1999; Schmidt, 2004). The margin offshore Namibia is characterised

as having characteristics of both a volcanic passive margin and a non-volcanic margin end members (Bauer et al., 2000; Gladchenko et al., 1998; Light et al., 1993). Five megasequences have been identified offshore Namibia, with each sequence coinciding with a significant phase of basin evolution (Bagguley & Prosser, 1999; Light et al., 1993). The phases include a pre-rift phase, two syn-rift extensional phases, followed by a transitional phase and a period of prolonged post-rift thermal subsidence or thermal sag (Bray et al., 1998). Syn-rift structures are timed to the Neocomian-Barremian with sag basin development during the Barremian-Aptian (Mello et al., 2013). Asymmetric rifting has resulted in significant variability in the sedimentary and subsidence history between the conjugate margins with this reflected in the nature of hydrocarbons discovered in these areas (Mello et al., 2011). The formation of the Walvis Ridge is contemporaneous with the extrusion of the Etendeka continental flood basalts and acted as a long-lived barrier to marine flow, creating restricted marine conditions to the north. These conditions promoted the formation of salt basins in the Albian-Aptian that are observed on both the West African and Brazilian margins (Berger et al., 1998; Davison et al., 2012). In the Lüderitz Basin multiple features such as seaward dipping reflectors (SDRs) and mass transport deposits (MTDs) can be observed (Torsvik et al., 2009). There are however no seamounts within 50 km from the study area, the outer limit for hydrothermal systems to extend from such a system (Hasterok et al., 2011; Sclater et al., 1980).

The neighbouring Orange and Walvis Basins both possess working petroleum systems with gas condensate discovered in the Kudu wells and oil in the Wingat well respectively (Fig 3.1b) (Intawong et al., 2015). The key source interval relevant for the Lüderitz Basin is the Aptian age Kudu shale (Fig 3.2d). The source maturity of this interval in the Lüderitz Basin is as yet uncertain.

Figure 3.2: (a) West-East transect displaying two-way travel time (TWT) seismic reflection structure in the Lüderitz Basin. Features visible include clinoforms in near shore section, with BSR, free gas zone (FGZ) below it highlighted by bright reflectors (associated with gas) and mass transport features in Tertiary section; (b) Inset map with sections displayed (see Fig. 3.1c for geographical context); (c) Close up of shallow Cenozoic sediments displaying MTD complexes. K-T boundary marked by intense polygonal faulting; (d) Close up of deeper Mesozoic section highlighting intrusive sills beneath a mounded platform like structure (believed to be a Barremian carbonate reef) overlain by Aptian age "Kudu shale" source rock interval; (e) Close up of SDRs at depth in the distal section of yellow highlighted 2D seismic line (Fig 3.2b)

3.2.2 Gas Hydrates & Bottom Simulating Reflectors

A BSR is traditionally considered as a continuous and coherent seismic event that cross-cuts the primary sedimentary features, whilst mimicking the morphology of the seabed (Calvès et al., 2008; Holbrook, 2001; Le et al., 2015; Paganoni et al., 2018). In shallow water, BSRs are usually due to multiple seabed-sea-surface reflections whilst in deep water the BSRs are much closer to the seabed than the seafloor multiple, requiring a different explanation. The 'soft' reflection of deep-water BSRs indicates an abrupt transition from relatively high- to low acoustic impedance. A BSR with such reverse polarity and near-parallelism relative to the seabed originates from the negative acoustic impedance contrast between partially frozen, gas-hydrate bearing sediment at the base of the GHSZ and the underlying zone of dissociated free gas and water bearing sediment (Kvenvolden & Lorenson, 2001; Paganoni et al., 2016). This variant of a BSR has been commonly noted in studies globally and is usually considered a sign of hydrate presence (Haacke et al., 2007; Shipley & Houston, 1979; Stoll & Bryan, 1979). Gas hydrates are naturally occurring substances formed when water in the subsurface freezes in a cubic, nonstoichiometric, crystallographic lattice structure, facilitated by the presence of methane and stabilised by hydrogen bonding (Kvenvolden & Barnard, 1982; Kvenvolden et al., 1984; Schicks, 2018; Sloan et al., 1998). Hydrates form under conditions of elevated pressure and low temperatures with abundant quantities of water and gas (Kvenvolden & Lorenson, 2001). Thus they are found both onshore in permafrost, and offshore in the shallow subsurface and on pipelines, leading to early study of hydrates focusing on their properties as a drilling and production hazard (Ruppel & Kessler, 2017; Schicks, 2018). Over 99% of global gas hydrates are methane hydrates (Ruppel and Kessler, 2017). The methane trapped within hydrate lattices is most often derived biogenically from the breakdown of organic matter in

the shallow subsurface, but may also contain thermogenic hydrocarbons, CO₂ etc (Taylor et al., 2000).

3.2.3 Heat Flow

Understanding heat flow is crucial to building reliable geological models of both the shallow and deep subsurface and has important implications for the exploration and development of natural resources such as petroleum (Tissot et al., 1987). Heat flow has traditionally been associated with tectonism and the thickness of the radiogenic crust. However mantle processes in continental margins also impact heat flow (Goutorbe et al., 2011). Heat from the mantle or primordial heat is one contributing factor to the thermal structure in sedimentary basins and is the deepest source of heat production (Hokstad et al., 2017). Mantle heat flow is estimated from the base of the crust, equivalent to the Moho (thus the prevalence of the 1330 °C isotherm as a reference point in traditional bottom up basin modelling workflows). When modelling, the depth to the lithosphere-asthenosphere boundary and Moho will predetermine the extent of the mantle heat contribution to heat flow (Hokstad et al., 2017). The other contribution to heat is in the form of radiogenic heat production within the rock column, primarily from the long-lived decay of radiogenic isotopes of thorium, uranium and potassium in sedimentary basins. The radiogenic heat production can be further subdivided into contribution from crystalline basement and that from sediments. Radiogenic elements are found in insignificant quantities in oceanic crust and lithospheric mantle, therefore the radiogenic heat input will be greatest in areas of continental crust and sediments (Allen & Allen, 2013; Hasterok, 2010). Basins located in the transitional zone between onshore and offshore regions tend to have considerable structural variability and thus as a consequence have been the least predictable for heat flow using global averages only (Hokstad et al., 2017; Jaupart et al., 2016). Though young ocean crust is particularly susceptible to hydrothermal

fluid circulation impacting heat flow, in the Lüderitz Basin this is not an issue due to the relative age of the underlying crust and proximity to the continent ocean boundary (Gladczenko et al., 1998; Lister, 1972).

Global coverage of heat flow data is not extensive, with surface heat flow data globally being limited relative to estimates of total heat output (Gosnold & Panda, 2002; Lucazeau, 2019; Macgregor, 2020). In the study area, the solitary heat flow data point is from ODP Site 1084 as shown in Fig 3.3. Reported values of heat flow in published literature are made either through direct measurement or through estimations based on crustal thickness and age (Davies, 2013; Davies & Davies, 2010). Such heat flow estimates can have a threefold basis with primary data from measured data points; in oceanic crustal settings, heat flow is based on crustal thickness to mitigate for measurement perturbation due to fluid flow; and finally in the absence of measurements an estimate can be made on the basis of geology. The Bullard (1939) method is commonly used to calculate heat flow from borehole data from the relation between temperature and the thermal resistance of the sediments (Bullard, 1939; Pribnow et al., 2000). For there to be a linear relationship between acoustic velocity and thermal conductivity conditions downhole must be conductive, steady state and with no internal heat sources. The latter is difficult as heat is introduced into the system during drilling from friction with the drill bit and the circulation of drilling fluids, thus necessitating time based corrections for the impact of drilling on local thermal regime.

Figure 3.3: Available heat flow data superimposed on the Namibian margin. Polygons represent mean heat flow estimates made at 1 degree grid resolution from geological models and borehole data (Davies, 2013). Point data is from the International Heat Flow Database and consists primarily of data from borehole measurements (Gosnold & Panda, 2002).

3.2.4 Conventional thermal data

Over large regions like continental margins, it is difficult to ensure high spatial resolution of thermal data from conventional techniques such as downhole temperature measurements

and gravity driven thermal probes (Phrampus et al., 2017). This is both a result of scarcity of boreholes and prohibitive expense. Heat flow derived from the seismic imaging of gas hydrates can be useful in areas where significant BWT fluctuation adversely affects the reliability of thermal probe data or where hard ground may prevent probe insertion (Hyndman et al., 2001; Phrampus et al., 2017). ODP thermal conductivity measurements on core samples from gas hydrate provinces are unreliable due to gas exsolution during recovery (Phrampus et al., 2017). This phenomenon depresses onboard thermal conductivity measurements. For the transient line source needle probe used in ODP studies to measure thermal conductivity it is important to note the orientation of the needle insertion relative to the sediment bedding direction as the thermal conductivity measurement is provided for a plane perpendicular to the needle axis (Pribnow et al., 2000). For shipboard temperature measurements temperature-time curves are subjectively fit to APC probe data (to restore to equilibrium temperatures and negate the effect of frictional heating upon insertion of the probe) (Grevemeyer & Villinger, 2001).

The Curie isotherm is a common subsurface thermal marker, thought to represent the bottom of the magnetic crust. It is a consequence of the Curie Point, the temperature above which certain materials lose their permanent magnetic properties. By using geophysical data such as remote sensing satellite magnetic data and the analysis of long wavelength magnetic anomalies, it becomes possible to estimate the depth limit to which magnetic sources are present (Rajaram et al., 2009). This may sometimes represent a petrophysical boundary (Langel & Hinze, 1998). The Curie isotherm is commonly considered to be $\sim 580^{\circ}\text{C}$ as this is the Curie Point temperature of magnetite, the most common magnetic mineral in the continental crust, especially in deeper regions (Frost & Shive, 1986). Thus, the depth corresponding to a lack of magnetism is likely at temperatures in excess of the Curie point of magnetite or a result of compositional changes leading to magnetite poor rocks at depth

(Beardsmore & Cull, 2001). However, this method simply defines a solitary subsurface isotherm over a great depth interval from the seabed, thus making any linear geothermal gradient calculated greatly approximated. Furthermore, for high resolution estimation of the Curie isotherm depth, regional scale gravity data would be required.

Global thermal data coverage may also suffer from spatial bias, as there tends to be a greater interest for scientists in areas of higher heat flow resulting in a greater concentration of data, with another potential driving factor being interest in areas with geothermal energy application (Davies, 2013).

3.3 Data

3.3.1 Seismic data

This study uses a combination of 2D and 3D multichannel, post-stack, time-migrated seismic reflection data from offshore Namibia, covering both the shallow- and deep-water sectors of the Lüderitz basin (Fig 3.1b & 3.1c). The seismic database is correlated with a single exploration well located on the continental shelf, in addition to ODP Site 1084 in the deep-water area.

The 2D seismic data were provided by Spectrum ASA and consists of two surveys conducted in 2006 and 2012 respectively, with further reprocessing in 2012 (to improve image quality in legacy data and to tie 2006 vintage seismic to newly shot 2012 seismic data), and a combined total line length of 752 km. The lines have a 4 ms two-way travel time (TWT) sample rate. The frequency range is 3 - 206 Hz (dominant frequency ~ 90 Hz) with a common mid-point (CMP) spacing of 12.5 m and a shot interval of 25 m. 2006 vintage 2D seismic data was collected with a streamer length of 8100 m while 2012 vintage 2D seismic data was collected with a streamer length of 10500 m.

The 3D seismic survey covers an area of 4150 km² and was acquired for Serica and partners by Polarcus in 2012 using *M/V Polarcus Nadia*. Primary objective of the survey was to establish prospectivity by mapping pinch out structures and a large channel feature in the study area. Streamer length was 8100 m with 50 m source separation of dual source (0.0695 m³) air guns. It is 80-fold with a 4 ms TWT sample rate and Inline spacing of 12.5 m and Xline spacing of 25 m. 3D pre-stack time migration was conducted by ION GXT. The isotropic frequency range for Kirchhoff pre-stack time migration (PreSTM) ranged between 3-110 Hz. All data were processed through stack and time migration. Velocity model building was done using two iterations of dense RMO auto-picking to create a smooth velocity model constrained by the geological horizons. Velocity model parameters of 4 ms sample interval, 9000 ms trace length and a 6000 m aperture. By parameterising the final velocity model (Fig. 3.4) for steep dips and high frequency gathers, the amplitude preserving preSTM resulted in high resolution image gathers.

Figure 3.4: West-East transect (Fig 3.1c) of seismic reflection volume in time domain overlain with interval velocities and K-T boundary highlighted. Velocities near seabed (indicated by the black line) are low (close to water velocity). Overall Tertiary section is characterised by low velocities. Velocity inversion seen near K-T boundary.

3.3.2 Well data

Well data included ODP Site 1084 and Norsk Hydro Exploration well 2513/8-1 (Fig 3.1b). The ODP borehole was drilled as part of ODP Leg 175 with the primary intention of documenting the migration of the Benguela Current along the South Atlantic West African Margin (Wefer et al., 1998). It is located in a water depth of 1992 m and targeted the downslope rim of the Lüderitz depositional basin. Useful subsurface borehole data included headspace gas analysis, gas chromatography results and core data.

The exploration well 2513/8-1 is situated on the shelf in a water depth of 243 m and targeted a Lower Cretaceous lobe in a thrust ramp graben before terminating in Barremian-Aptian age volcanic rocks at a total depth of 2553 m. Some sparse bottom hole temperature (BHT) data points from this well provide the only available calibration for the temperature estimation workflow.

3.4 Method

Figure 3.5: Schematic summary of the steps involved as part of the seismic led temperature estimation methodology explored in this paper.

The temperature estimation workflow utilised in this study is outlined in Fig 3.5 and described below. The entirety of the workflow has been developed and tested using commercial software developed for use in the petroleum industry (Schlumberger Petrel).

The gas hydrate stability field can be utilised to estimate the temperature at the base of the zone of stable gas hydrates, demarcated on seismic by a bottom simulating reflector (Dickens & Quinby-Hunt, 1994; Lu & Sultan, 2008; Sloan et al., 1998). This in turn allows a shallow geothermal gradient across the GHSZ to be estimated and surface heatflow to be estimated (Minshull, 2011; Priyanto, 2018). The stability conditions are controlled in part by the geochemical properties of the fluids available to form clathrate hydrates, which in frontier settings with limited ground truthing are generally assumed to be average sea-water salinity (33.5 ‰) and pure methane (Sloan et al., 1998). Pore fluid pressure conditions are generally assumed to be hydrostatic, equivalent to $0.0101 \text{ MPa m}^{-1}$. The following relationship (Eq. 1) as defined by (Dickens & Quinby-Hunt, 1994) describes methane hydrate stability:

Equation 1:
$$\frac{1}{T_{BSR}} = 3.79 \times 10^{-3} - 2.83 \times 10^{-4}(\log P)$$

where T_{BSR} is temperature at the base of GHSZ (K); and P is the corresponding pressure (MPa). Assuming hydrostatic pressure at the BSR depth, pressure is simply a function of depth below mean sea level. It is possible then to rearrange in terms of depth below sea level. Thus, temperature at the base of the hydrate stability zone has been established:

Equation 2:
$$T_{BSR} = ((3.79 \times 10^{-3} - 2.83 \times 10^{-4}(\log(\rho \times g \times Z_{BSR})))^{-1}) - 273$$

Where T_{BSR} is the temperature at GHSZ (°C); ρ is density (kg m^{-3}) (of seawater); g is acceleration due to gravity (m s^{-2}) and Z_{BSR} is the depth (m) of the BSR. It must be noted that this is a minimum temperature estimate based on assumed stability field conditions (Dickens, 2001).

Seafloor temperature can be acquired from direct measurements or open source datasets such as the National Oceanic and Atmospheric Administration (NOAA) World Ocean Atlas

(WOA) (Boyer et al., 2005). Annualised mean data points for water column temperatures correspond to standard NOAA depth intervals. To simulate the hydrothermal gradient at this location, a regression was applied to these data points. A solitary regression fit for the data points representing the entire water column in this location will have discrepancies at various depth intervals. Using such a regression to model seafloor temperature can impact the validity of the results of the overall temperature prediction workflow. However, compartmentalising the water column into discrete depth intervals (epipelagic, mesopelagic and bathypelagic zones respectively), certain trends are found to be common globally within such intervals. It was thus seen that far better regression fits were observed corresponding to each segment, with the average misfit from this approach amounting to ± 0.4 °C across the water column (see Fig. 3.8b).

$$\begin{aligned} \text{Equation 3: } T_{SEABED} &= (-1.919 \ln Z + 21.899) && \text{if } Z \leq 200 \\ T_{SEABED} &= 525.65Z^{-0.714} && \text{if } 200 < Z < 1000 \\ T_{SEABED} &= -0.0007Z + 4.4905 && \text{if } Z \geq 1000 \end{aligned}$$

where T_{SEABED} is the modelled hydrothermal gradient temperature (°C) and Z is seabed depth (m).

Given T_{SEABED} , Z_{SEABED} AND T_{BSR} , Z_{BSR} at any geographical locality, then the geothermal gradient (dT/dZ) across the GHSZ at that locality is given by the following relationship.

$$\text{Equation 4: } \frac{dT}{dZ} GHSZ = \frac{T_{BSR} - T_{SEABED}}{Z_{BSR} - Z_{SEABED}}$$

Where dT/dZ is geothermal gradient (°C km⁻¹); T_{BSR} is temperature at BSR (°C); T_{SEABED} is seabed temperature (°C); Z_{BSR} is depth of BSR (km); Z_{SEABED} is seafloor depth (km).

Fourier's Law of heat conduction links heat flow, thermal conductivity and thermal gradient. It is given by the following relationship.

$$\text{Equation 5: } Q = k \times \frac{dT}{dZ}$$

Where Q is heat flow (mWm^{-2}); k is thermal conductivity ($\text{W m}^{-1} \text{K}^{-1}$) (see Section 3.4.1) and dT/dZ is geothermal gradient ($^{\circ}\text{C km}^{-1}$).

Fourier's Law of heat conduction (Eq. 5) is crucial to understanding the interplay between heat flow, thermal conductivity and geothermal gradient. Establishing a shallow linear geothermal gradient using BSRs is well established (Calvès et al., 2010; Serié et al., 2017) and studies have extrapolated this shallow geotherm for traditional basin modelling workflows. This however does not consider the thermal conductivity structure of the subsurface and how it might be possible to utilise seismic reflection velocity data to do so.

3.4.1 Thermal conductivity estimation

Thermal conductivity is a measure of how well heat is conducted through a material (Gu et al., 2017). It characterises the heat transfer capability as a result of temperature gradient (Mielke et al., 2017). Difficulty associated with measuring thermal conductivity in boreholes arise from poor contact between the measuring tool and the borehole wall (Horai, 1982). Thus, considerable attention has been devoted to determining methods for estimating thermal conductivity through more easily acquired secondary data such as seismic velocity measurements. Experimental studies have shown that primary controls on thermal conductivity include mineral composition, porosity and fractures (Gegenhuber & Schoen, 2012). Seismic wave velocity is also largely controlled by the same factors. Early work by (Horai, 1982) sought to correlate thermal conductivity with other physical properties such as water content, bulk density, porosity and compressional sound wave velocity. The direct approach involves deriving thermal conductivity from physical properties via empirical relationships (Zamora et al., 1993). Estimates of thermal conductivity computed directly from conventional wireline data can be accurate within $0.2 - 0.3 \text{ W m}^{-1} \text{K}^{-1}$ when derived using empirical relationships from sonic velocity data (Hartmann et al., 2005). Such a direct

approach has been utilised in this work using experimental data from existing correlation studies (Brigaud et al., 1990; Brigaud & Vasseur, 1989; Esteban et al., 2015; Griffiths et al., 1992; Gunn et al., 2005; Kukkonen & Peltoniemi, 1998; Francis Lucazeau et al., 2004; Mielke et al., 2017; Popov et al., 2003; Popov et al., 1999).

Experimental data can vary in terms of the conditions under which it was collected. Binary parameterisation of the experimental datasets allows characterisation of data points collected under similar parameters/conditions. Parameters include the manner in which thermal conductivity measurements were made (transient or steady state); the tool by which P wave velocity is measured for the samples; the geographical location of the data; the sample type (core or not); the conditions under which the measurements were made; and sample condition (wet or dry). Most studies measured thermal conductivity using the optical scanning method developed by (Popov et al., 1999). There are fewer instances in the source datasets of the use of the divided bar method of measuring thermal conductivity (Evans, 1977; Hyndman & Jolivet, 1976). A decision was made to only consider the wet samples from these studies as our case study is in deep water and thus fully saturated with water, gas and/or gas hydrate. In dry samples, the contribution to thermal conductivity due to lithological heterogeneities (matrix properties) can be masked by the stronger influence of porosity (Hartmann et al., 2005). In contrast wet samples reflect the impact of porosity and lithological variations.

The range of samples included in our fits cover a wide range of lithologies, including sandstones, limestones, granites, basalts, marble to name a few (Boulanouar et al., 2013; Esteban et al., 2015; Grevemeyer & Villinger, 2001; Gu et al., 2017; Hartmann et al., 2005; Jorand et al., 2015; Mielke et al., 2017). In so doing it is hoped that the resulting empirical relationship will best apply to the broadest possible range of rock types that can be expected subsurface across the study area. Most measurements have been taken at ambient pressure

and temperature conditions. It must be noted though that variables within the sample set (Fig. 3.6) include and are not limited to the porosity (arising from cracks for example). Fractures are known to reduce both P wave velocities and thermal conductivity (Zamora et al., 1993).

A regression through the filtered experimental data points taken from the aforementioned studies gives the following empirical relationship for thermal conductivity:

Equation 6: $k_V = (0.001 \times V_P) - 0.5071$

Where k_V is thermal conductivity from velocity ($\text{W m}^{-1} \text{K}^{-1}$) and V_P is P wave velocity (m s^{-1})

Figure 3.6: Empirical velocity to thermal conductivity transform utilising experimental datasets from published literature. These measurements are made on samples in laboratory conditions and represent a wide range of lithologies. Furthermore, only results from wet sample measurements are displayed, as the transform will be applied in the shallow subsurface where there is very likely to be fluid fill (for example the GHSZ). Measurements were made using transient method (optical scanning equipment).

Certain trends are evident in the cross plot of sample data in Fig. 3.6. Due to the lack of salt encountered in the study area, there is a lack of sample points in the expected high conductivities associated with salt (Esteban et al., 2015). The regression is anchored by the

large cluster of points associated with the Grevenmeyer & Villinger (2001) data. The Hartmann et al. (2005) and Gu et al. (2017) samples are parallel to the best fit regression.

Seismic P wave velocity within the area is converted to thermal conductivity (k_v) using the thermal conductivity relationship (Eq. 6), with velocity averaged down to the depth of the BSR, Z_{BSR} . The variation in thermal conductivity with depth can be overlain on a 3D seismic reflection dataset in this manner. Using the depth of the BSR, Z_{BSR} (Fig. 3.9a), determined on reflection seismic data, the hydrate stability field can be utilised to compute the temperature at this phase boundary (Fig. 3.9b) for the base of the GHSZ (using Eq. 2). Temperature at the seabed is known from the hydrothermal gradient (given by Eq. 3). A shallow geothermal gradient may thus be computed between seabed and BSR (Eq. 4). As thermal conductivity has been derived from acoustic velocity data, and with shallow geothermal gradient also available, it becomes possible to reapply Fourier's Law (Eq. 5) to derive heat flow for this area. Estimating the shallow geotherm and heat flow along the full extent of a BSR helps eliminate the bias in heat flow distribution from direct measurements taken at discrete locations (Shankar & Riedel, 2013). This BSR derived heat flow proxy is used in conjunction with the bulk thermal conductivity volume to generate a volume of average geothermal gradient for the bulk volume (rearranging Eq. 5).

Temperature below the seafloor can be summarised as being a function of the depth below the seafloor and the aforementioned average geothermal gradient. It follows that an estimate of temperature may be arrived at through this simple relationship where the temperature at any given depth point is given by multiplying the average geothermal gradient against the depth to that point:

Equation 7:
$$T = T_{SEABED} + \left(\frac{dT}{dZ} \times Z_{SUBSURFACE} \right)$$

where T is predicted temperature ($^{\circ}\text{C}$); T_{SEABED} is the temperature at seabed ($^{\circ}\text{C}$); dT/dZ is the average geothermal gradient ($^{\circ}\text{C km}^{-1}$); and $Z_{SUBSURFACE}$ is the subsurface depth (km). Seabed

temperature (Fig. 3.8a) is added to account for the effect of the hydrothermal gradient on the subsurface temperatures.

As the average geothermal gradient is only valid for the subsurface and due to the seismic input volume containing the water column it becomes necessary to negate the latter. Without flattening the volume to the seabed, it is instead possible to use the seabed depth map to derive a depth volume relative to seabed depth.

Equation 8: $Z_{SUBSURFACE} = Z - Z_{SEABED}$

where $Z_{SUBSURFACE}$ is the subsurface depth (km); Z is the absolute depth (km); and Z_{SEABED} is the seabed depth (km).

The steps outlined above are all possible using basic functions available within the Petrel seismic interpretation suite. Should there be a discrepancy between the seismic reflection volume and the interval velocity volume, it becomes difficult to convolve instantaneous geothermal gradient versus the subsurface depth volume. Discrepancies may include sampling rate; inline and crossline spacing; or there might be a misalignment of the two volumes. In this case a geo-cellular model, traditionally utilised in reservoir modelling, may be developed for this workflow. A pillar grid corresponding to the extent of the seismic survey is built. The original seismic reflection time and seismic reflection velocity data can be resampled into the pillar grid. It must be noted that resampling the original data can result in a loss of fidelity from the algorithm used and the size of the voxels comprising the model. Here, an averaging algorithm is used for voxel sizes of 50 m * 50 m * 10 m. An average of all traces corresponding to the voxel are assigned. Compared to a like for like resampling, this algorithm is computationally less intensive. The advantage of using such a pillar grid is that computation of the various properties such as velocity derived thermal conductivity (k_v) become easier. It is also easier to model pseudo boreholes in this manner.

3.4.2 Uncertainty modelling

An attempt to model uncertainty was made following the use of 95% confidence interval method as used by (Phrampus et al., 2017) to derive bounds for both the heat flow proxy from BSR and the overall temperature prediction. The approach to calculating these bounds can be considered modular for the two aforementioned predicted thermal properties, with the same workflow (Fig. 3.5) also used here but with an upper bound and lower bound approach for each step as shown in Table 3.1. For example, to model the lower bound of the shallow heat flow proxy, firstly the lower bound of RMS of interval velocity across the GHSZ is used to domain convert the TWT BSR pick. This has the effect of varying the BSR in depth, to a shallower depth as a result of the lower interval velocity selected which in turn would result in a lower temperature for the BSR using the hydrate stability field relationship described previously. It must be noted that the hydrate phase composition is not varied and that the pressure field is unaltered from previous modelling. Similarly, the seabed depth and temperature are considered unchanged. A lower bound for geothermal gradient is arrived at using these conditions. Using the 1D approximation of Fourier's law (Eq. 5) this lower bound geothermal gradient is convolved with the lower bound regression for thermal conductivity from velocity separate from that discussed in Section 3.4.1 but based on the same 95% confidence interval. This results in the lower bound of the heat flow estimate from the BSR. Using the opposite bound of the various aforementioned component steps helps arrive at the upper bound for heat flow. The bounds for the temperature prediction can be simplified to varying the bulk thermal conductivity volume and conditioning the model with the heat flow from BSR bounds arrived at. In doing so an envelope of temperatures representing the spread of values possible using 95% confidence for all input parameters.

Table 3.1: Parameters for BSR derived heat flow bounds

Sediment velocity (m s⁻¹)	Hydrate phase	Thermal conductivity (W m⁻¹ K⁻¹)	Pressure conditions	Seabed temperature	Heat flow bound
Minimum	Pure methane & seawater	Minimum	Hydrostatic	Modelled hydrothermal gradient	Minimum
Maximum	Pure methane & seawater	Maximum	Hydrostatic	Modelled hydrothermal gradient	Maximum

3.5 Results

The BSR observed in the area has been mapped across the NW and SW quadrants of the 3D reflection seismic coverage (Fig. 3.7). Though the full extent of the visible BSR was mapped, only the extent corresponding to the highest confidence seismic picks are displayed as the clarity of the BSR degrades towards the edges (Fig. 3.7c). This would introduce anomalous artefacts and edge effects and hence are excluded. It is this high confidence extent of the BSR that is referred to in the following sections unless otherwise specified. The BSRs are found to have opposite seismic reflection polarity to the seabed reflection indicating the likelihood of gas hydrate above free gas (Kretschmer et al., 2015) (Fig. 3.7a). Though there is no record of hydrates from ODP Site 1084, high amplitude reflections are observed to occur in close proximity below the BSR, characteristic of the presence of trapped gas. Temperature at BSR depth and the phase relationship used to determine this is shown in Fig. 3.9.

Figure 3.7: (a) Close up of BSR (red dashed line) with acoustic impedance (AI) contrasts shown at seabed and BSR. Vertical features have chimney like appearance and pass through the FGZ and extend to seabed; (b) Red marker for section displayed in (a); (c) BSR depth map; (d) Thickness map of the GHSZ. Areas shown for (c & d) correspond to high confidence BSR area with extent of mapped BSR represented by black polygon and displayed for reference. The hydrate stability zone has an average thickness of 184 m as observed within the study area (Fig. 3.7d). The cumulative area of both the mapped BSRs is $0.941 \times 10^9 \text{ m}^2$. Assuming all the sediment above the BSRs contain gas hydrate, a typical hydrate saturation of 10 % (Waite et al., 2009) would yield a potential methane hydrate volume of $1.73 \times 10^{10} \text{ m}^3$.

Figure 3.8: (a) Seabed temperature mapped using a synthetic hydrothermal gradient with 200m bathymetric contour markers (b) modelled after NOAA WOA annualised mean data for the most recent decadal period between 2005-2012, mapped at a 1° grid resolution (Becker et al., 2009; Locarnini et al., 2013).

Figure 3.9: (a) Temperature at the BSR mapped on high confidence area. Full extent of BSR demarcated by black polygon. (b) Hydrate stability field for a pure methane-seawater system for the study area. Adapted from (Dickens & Quinby-Hunt, 1994; Lu & Sultan, 2008)

Neither the exploration well nor ODP borehole 1084 fall within the bounds of the thermal model. As a result, direct calibration is not possible. However well 2513/8-1 contains BHT information that may provide some calibration for the predicted results. Pseudo boreholes provide a means of simulating 2513/8-1 at a comparable location along strike (Fig. 3.10b&c). P1 is projected into the study area following bathymetric contours (Fig. 3.8a) as close as possible along strike from 2513/8-1, in order to maintain structural parity. The results are shown in (Fig. 3.12). BHT recordings typically are lower than actual formation temperature due to cooling effect of circulating fluids in a borehole and thus they must be corrected (Deming, 1989). There are insufficient points for a Horner correction (Bonté et al., 2012; Horner, 1951) to be applied and hence a rudimentary correction is made for time since circulation (see <https://www.zetaware.com/utilities/bht/timesince.html> first accessed August 2018). The predicted temperatures are between 17 and 26% higher than the corrected BHT (Fig. 3.12a). On seismic data it was evident that there is a deeply incised canyon like structure trending NE – SW that can be seen in the north-eastern most extent of the seismic volume (Wanke & Toirac-proenza, 2018). This corresponds to the location of P1, which is seen to intersect the channel fill structures of this canyon. It becomes evident then that though P1 was projected into the seismic volume maintaining bathymetric parity, in the subsurface, due to the occurrence of this channel like geometry, it is not possible to maintain stratigraphic parity to 2513/8-1. This is surmised to be the primary factor for the misfit with BHT seen.

Further pseudo-wells (T1 – 3) were modelled to examine the change in thermal profile moving from the proximal section to the distal part of the study area (Fig. 3.10a). The results of these are displayed in Fig. 3.12. They also display what the thermal profile in these boreholes would be like should a typical geothermal gradient of $30\text{ }^{\circ}\text{C km}^{-1}$ were applied linearly from seabed, and a higher geothermal gradient of $40\text{ }^{\circ}\text{C km}^{-1}$ was applied in a similar manner too. The temperature window considered prospective for reservoirs in present day has been referred

to as the Golden Zone (60 – 120 °C). It becomes apparent then that the varying geothermal gradient with depth of the proposed model would significantly alter the subsurface depth at which the Golden Zone would begin and end in comparison to the typical linear geothermal gradients that are often considered in a traditional basin modelling workflow. Analysing the geothermal gradient between these pseudo-wells it is seen that in the proximal section (T1) there is a much steeper drop off (~ 57.1 °C km⁻¹ in the uppermost 800 m to 15 °C km⁻¹ in the deepest 1000 m) compared to the intermediate (T2) and deeper sections (T3). The spread of isotherms in a dip section (Fig. 3.10a) reflects this. Isotherm spacing is even in the Mesozoic section moving into deeper water. However, in the proximal end corresponding to minimal Tertiary cover, there is observed the greatest divergence between isotherms in Mesozoic sediment. Temperature for the Aptian ‘Kudu shale’ source rock in the region has also been mapped (Fig. 3.11).

Below the northern BSR (Fig. 3.7a) the effects of gas blanking were observed in the seismic reflection data. A Root Mean Squared (RMS) velocity extraction reveals anomalously low values within this area (Fig. 3.10c). Borehole T4 was modelled targeting this area. The results of this borehole are consistent with the deep-water borehole T3 with similar geothermal gradient at each 1000 m interval between the two boreholes.

Figure 3.10: (a) Depth profile with temperature predicted from seismic model overlain. Boreholes corresponding to shallow, intermediate and deep water are marked. (b) Map outlining the modelled pseudo boreholes within the area. (c) RMS velocity extraction of interval velocities (for interval up to 2 s below seabed) highlighting the zone of low velocities encountered below the Northern BSR. Borehole T4 specifically targets this.

The base of the Aptian source rock of key interest in the study area occurs above the mounded structure referred to as Prospect B (Fig 3.2d). The thermal model produced was used to interrogate the predicted present-day temperature for the base of the source rock interval as shown in Fig 3.11. The temperature ranged between 93.2 – 157.2 °C for a depth range of 3400 – 5400 mbsl.

Figure 3.11: Thermal map of top of mounded reef like structure focused around 4300 m closing contour (Fig 3.2d) with 200 m contour intervals.

Figure 3.12 Modelled borehole results for subsurface temperature with Golden Zone interval overlain for reference. (a) Thermal profile for pseudo borehole P1 simulating 2513/8-1 with corrected and uncorrected BHT readings. 95% confidence upper and lower bounds are also displayed. (b) Thermal profile for boreholes T1-T4. (c) T1 shallow water thermal profile with modelled linear geothermal gradients. (d) T2 intermediate water depth thermal profile with modelled linear geothermal gradients. (e) T3 deep water thermal profile with modelled linear geothermal gradients. (c-e) Modelling subsurface temperature with typical linear geothermal gradients highlights the variability in depth expected for the Golden Zone.

3.6 Discussion

3.6.1 Uncertainty

In a quantitative workflow such as the one discussed in the paper, there are multiple avenues for uncertainty in the constituent steps. Previous literature includes attempts to quantify the uncertainty in predictions using a BSR derived geothermal gradient (5 – 35%) and heat flow (10 – 50%) (Grevemeyer & Villinger, 2001). Such attempts have usually quantified uncertainty for the component steps rather than the compound uncertainty for the entire process. For this work, with a lack of well data for ground truthing, the temperature estimation bounds for 95% confidence were used to give an idea of the range within which the estimates can vary. It is important to note the impact of variability in input factors for the component steps. For example, results from the Blake Ridge show that actual temperatures at the BSR depth could be between 0.5 – 2.9 °C lower than the temperature predicted by the hydrate phase relationship for that particular depth and pressure (Wood & Ruppel, 2000). This implies that a significant source of uncertainty in the thermal modelling could result from the assumptions made about the conditions at the base of the GHSZ. As stated earlier, an assumption has been made on the lattice fluid and trapped gas mix for the hydrate zone in the absence of direct piston core sampling. Varying gas compositions can vary the hydrate stability and thus alter the temperature at the bottom simulating reflector (Chand et al., 2008). The prevalence of methane hydrates globally leads us to assume it is the most likely composition of the hydrates in the study area.

Bottom water temperature (BWT) fluctuations, both the magnitude and time scale for which they occur provide another element of uncertainty. It must be noted that the strong Benguela Current flows along the Namibian margin in this area and it is difficult to directly factor in the impact that this may have on the modelling. However, the data used to generate a model of the hydrothermal gradient in the area utilised NOAA data that have been averaged annually over an eight-year period. It is thus hoped that any temporal perturbations of BWT are accounted for by the dataset.

The quality of the initial velocity model is another source of uncertainty. As thermal conductivity is derived from it using a direct empirical relationship, any anomalies in the existing velocity model or velocity data will be translated into the derived properties. From the low spread of RMS interval velocities for the GHSZ it is apparent the application of a default 1500 ms^{-1} velocity above seabed during the velocity model building stage results in a heavily smoothed velocity model. This is expected to be reflected in the nature of the temperature profile generated using velocities as input.

In the absence of a reliable heat flow recording for this area, a BSR derived heat flow proxy has been used. This is a shallow heat flow as it uses an average velocity derived thermal conductivity and geothermal gradient valid within the GHSZ (Eq. 5). Unlike in traditional basin modelling the radiogenic heat production of the rock column has not been integrated. Instead this solitary heat flow proxy has been used to condition the model for an average geothermal gradient. Though hydrothermal fluid circulation in the subsurface can also greatly alter heat flow, both vertically and laterally, the study area is likely to be minimally impacted in this regard. As the study area is sufficiently distant from a neighbouring seamount to negate the convective and advective heat flow impact of hydrothermal fluid circulation, heat transport in this area is predominantly conductive. Therefore, the assumption is of limited lateral heat flow variability, which is backed by the BSR-derived thermal gradients and derivative heat flow

estimates. An idea of the uncertainty of the heat flow derived in this manner has been computed using the method shown in (Phrampus et al., 2017). Heat flow is found to range between 46.2 – 76.2 mWm⁻², with the weighted mean for the heat flow used for computation of the temperature model equal to 63.8 mWm⁻². The lower bound of the derived range is consistent with results from (Macgregor, 2020) while the upper bound would be in line with the preferred prediction from the global map in Lucazeau (2019). The weighted mean is interestingly consistent with the continental margin heat flow mean reported by (Davies, 2013). The heat flow range given by the bounds is consistent with observational data and estimations of heat flow from age relationships corresponding to this area (Hamza & Vieira, 2012).

3.6.2 Implications

As stated previously, the source maturity of the Aptian Kudu shale interval in the Lüderitz Basin is a key unknown in terms of the petroleum systems elements. With the thermal modelling workflow indicating an average temperature of 133.5 °C across the top of this Barremian structure (Fig. 3.11), the base of the overlying Kudu shale source rock immediately above would therefore lie in the gas generation window (Bjørlykke et al., 1989). This is consistent with the nearby Kudu fields which produce gas condensate from the same Aptian source interval. The results would suggest then that the Lüderitz Basin has an improved prospectivity outlook with the potential for a working hydrocarbon system with gas charged reservoirs.

It was possible in this study to estimate present day temperature at key subsurface target depths in a frontier setting in the absence of any substantive well control. The workflow presented would enable seismic operators to utilise the data libraries of seismic reflection and velocity data available to them to generate present day estimations of subsurface

temperature in a non-invasive manner, prior to an expensive drilling campaign. It is hoped that this would help streamline petroleum systems analysis and provide an additional dataset for basin modellers to use with the aim of decreasing the uncertainty with which frontier regions are explored.

3.7 Conclusions

The model proposed in this study is a simple and robust methodology for estimation of present-day subsurface temperature in frontier areas lacking borehole control for temperatures. It makes use of readily available seismic reflection and velocity data in a workflow developed on an industry standard software suite. It highlights how existing workflows for BSR derived heat flow may be combined with existing experimental thermal conductivity and velocity data for various lithologies to develop an empirical transform that may be applied to seismic velocity models. Given thermal conductivity and P wave velocity have sensitivity to similar parameters, this methodology would allow the user to examine the vertical and lateral variability in thermal properties in a frontier basin especially when high-quality pre-SDM and FWI velocity models are available. The results of the case study documented here suggest that the main prospect lies just below the golden zone and that sources rocks are in the generative window.

3.8 References

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4. Seismic characterization of thermal regime: a Blake Ridge study

Key Points:

- Non-invasive thermal regime characterization methodology utilizing seismic data.
- Testing in the Blake Ridge hydrate province expands subsurface temperature profile beyond existing data.
- Borehole velocity data has been used to condition an empirical subsurface thermal conductivity model.

4.1 Abstract

Constraining the subsurface thermal regime is of importance not just to the offshore hydrocarbon exploration industry but also for understanding the geothermal regime in context of microbiological activity. This regime is tested through the use of seismic data to noninvasively estimate subsurface temperatures through the identification of bottom simulating reflectors (BSRs) at the base gas hydrate stability zone (GHSZ) to mark out an isotherm. This methodology is applied to the Blake Ridge, offshore east coast USA, where ODP Leg 164 boreholes provide temperature data required for thermal model constraints. 3D thermal modelling using reflection seismic data is used to examine the lateral variability of the shallow thermal regime while 1D thermal modelling is applied to ODP Sites 994, 995 and 997. The resulting estimated subsurface temperature profiles had a margin of error of 13.9% compared to in situ temperature measurements recorded from the boreholes. This method of thermal modelling could significantly expand the application of thermal data from ODP sites to areas covered by seismic data, which would considerably benefit researchers worldwide in industry and academia.

4.1.1 Plain Language Summary

The Blake Ridge has extensively been studied for gas hydrates. As such it serves as an excellent location to test a seismic led approach to subsurface thermal regime characterization that the authors previously developed using data from the Lüderitz Basin, offshore Namibia.

4.1.2 Acronyms

- 1D – One dimensional
- 2D – Two dimensional
- 3D – Three dimensional

- APC – Advanced Pressure Core
- BSR – Bottom Simulating Reflector
- BWT – Bottom Water Temperature
- CMP – Common Mid Point
- DVTP – Davis Villinger Temperature Probe
- GEBCO – General Bathymetric Chart of Oceans
- GHSZ – Gas Hydrate Stability Zone
- mbsf – metres below sea floor
- NOAA – National Oceanic and Atmospheric Administration
- ODP – Ocean Drilling Program
- PCS – Pressure Core Sampler
- PSTM – Post Stack Time Migrated
- RCB – Rotary Core Barrel
- RMSE – Root Mean Squared Error
- SWIT – Sediment Water Interface Temperature
- TWT – Two Way Travel Time
- VSP – Vertical Seismic Profile
- WBUC – Western Boundary Undercurrent
- WHOI – Woods Hole Oceanographic Institute
- WOA – World Ocean Atlas
- WSTP – Water Sampler Temperature Probe
- XCB – Extended Core Barrel

4.2 Introduction

Constraining the subsurface thermal regime allows the estimation of heat available for low temperature diagenetic processes and microbial incubation (Fuchs & Balling, 2016; Purkamo et al., 2020). It also allows the evaluation of advection in local heat transport. Understanding the distribution of temperature in the subsurface is important to the geothermal energy industry and in particular the energy sector, for hydrocarbon generation is greatly dependent on temperature conditions (Bonté et al., 2012; Hunt, 1984; Thompson, 1979). Present day thermal data in the subsurface is traditionally acquired using measurement probes lowered into a borehole (Lucazeau et al., 2004). Ocean Drilling Program (ODP) borehole logging data often contains a thermal data suite, characterizing parameters such as temperature, geothermal gradient, thermal conductivity and heat flow (Popov et al., 1999; Pribnow et al., 2000). This presents a globally available subsurface thermal database accessible for researchers worldwide. However, in the absence of boreholes, it becomes difficult to determine the thermal regime in offshore domains. Seismic data enables visualization of subsurface physical features, but it can also be used to derive thermal data. Phenomena known as bottom simulating reflectors (BSRs) occur at the phase boundary for stable gas hydrate, and represent an isotherm due to hydrate stability being controlled primarily by temperature and pressure conditions (Serié et al., 2017; Shankar et al., 2014; Yamano et al., 1982). The Blake Ridge has been studied for nearly thirty years as an area of interest for gas hydrate research (Paull & Dillon, 1981). The area contains numerous indicators on seismic for the presence of gas hydrate including most importantly, BSRs. The authors have previously developed a methodology to determine present day subsurface temperatures from seismic data on a continental margin with a visible BSR (Sarkar & Huuse, 2021b). Testing this methodology in the Blake Ridge allows calibration of the temperature modelling process against the abundant thermal data records published as part of ODP Leg 164.

4.2.1 Geological setting

The Blake Ridge is located on the southeastern US passive margin offshore the South Carolina coast (Fig. 4.1a). This physiographic feature is a Neogene and Quaternary sediment drift deposit formed from the erosion of the Blake Plateau (Burwicz & Rüpke, 2019; Wood & Ruppel, 2000). Evidence for the effects of sediment reworking through bottom currents is seen from sediment wave fields and erosional scouring of the seabed on the southern flank of the Blake Ridge (Fig. 4.1b) (Burwicz & Rüpke, 2019; Hornbach et al., 2008). The Western boundary undercurrent (WBUC) sweeps southward along the continental slope encountered here and mixes with the Gulf Stream at bottom water depths. This acts as a control on topography (Hornbach et al., 2003). Drilling results reveal the sediments in this area to be homogeneous and dominated by clays ranging from nannofossil clays, claystones and fine grained mudstones (Holbrook et al., 1996). Sediments at Blake Ridge are rich in organic carbon with organic matter having a mainly marine signature (Paull et al., 2000). Evidence from recovered cores indicates sedimentation rates were progressively higher going back to the Pliocene (Burwicz & Rüpke, 2019).

Drilling in this area down to a maximum depth of 750 m below the sea floor found intermittent filling of the pore space with hydrates (Paull & Matsumoto, 2000). The occurrence of hydrates has been noted in some instances as greyish concentrated nodules at Site 994, although in Site 995, it is fine grained and dispersed in the host sediment (Paull et al., 1996c).

The sediment homogeneity in the Blake Ridge (Fig. 4.2a), combined with the tectonic inactivity, stable seafloor conditions and lack of structural complexity have made this area attractive for the study of the impact of gas hydrate presence on seismic response (Hornbach et al., 2008).

Figure 4.1: (a) Bathymetric map highlighting Blake Ridge study area offshore Carolina coastline with extent of the study area, mapped BSR, and ODP Leg 164 Sites for reference. Erosional scouring of seabed coincides with buried sediment wavefield. ODP Site 997 is located on the crest of the ridge structure. (b) Inset map of eastern US seaboard indicating study area location in context of published BSR extent. International heat flow database points both onshore and offshore give an idea of thermal data coverage in the literature. Adapted from Becker et al., 2009; Gardner, 2013; Hornbach et al., 2003; Paull & Matsumoto, 2000; Ryan et al., 2009

4.2.2 Gas hydrates and bottom simulating reflectors at the Blake Ridge

Gas hydrates are naturally occurring frozen crystallographic lattices of ice trapping a guest gas molecule (Kvenvolden, 1985; Sloan et al., 1998). Gas hydrates form under elevated pressure and low temperature conditions, thus being observed onshore in permafrost at high latitudes as well as in the marine domain (Kvenvolden & Lorenson, 2001; Ruppel & Kessler, 2017). Marine gas hydrate deposits are primarily located along continental margins at water depths exceeding ~300 m and sufficiently low bottom water temperature. Gas hydrates form

clathrate structures which are characterized into three subtypes (Sassen & MacDonald, 1994). Gas hydrates at Blake Ridge are mainly structure I hydrates, the most commonly occurring variety. The gases trapped within these clathrate cages are mostly hydrocarbons, with cage size determining the length of the carbon chain that can be accommodated (McConnell & Kendall, 2002). Methane is the most common trapped gas within gas hydrates and this is also found to be the case in the Blake Ridge (Paull & Dillon, 2001). Minor quantities of other gases such as carbon dioxide may also be found. The methane is either sourced locally from the biogenic breakdown of organic matter in the shallow subsurface or thermogenically from deeper sources (Sassen et al., 2001; Serié et al., 2017). Trapped gases have an isotopic and molecular signature suggestive of a microbial origin for hydrocarbon molecules (Burwicz & Rüpké, 2019; Paull et al., 1996a). Chloride ion excursions measured from pore water recovered from sediment core samples are a strong geochemical indicator for the presence of gas hydrates (Holbrook et al., 1996). The occurrence of gas hydrate zones across the Blake Ridge is supported by the similarity in chloride profiles with characteristic negative excursions across all three ODP Leg 164 sites (Paull et al., 1996a).

Geophysical detection of gas hydrates is commonly done through the identification of markers known as BSRs, which are often considered the most robust evidence of gas hydrate presence (Shipley & Houston, 1979). A BSR is a seismic event that mimics seafloor morphology whilst appearing to cross cut sedimentary strata (Calvès et al., 2008; Holbrook, 2001; Paganoni et al., 2016). The depth at which the BSR is observed is where the temperature is in excess of the hydrate stability field, causing the frozen gas hydrate to break down to water and gas (Hornbach et al., 2003). As such the BSR is attributed as a marker for the base of the gas hydrate stability zone GHSZ (Fig. 4.2b) (Haacke et al., 2007). It is distinct in having reverse seismic polarity to the seabed as a consequence of a reduction in acoustic impedance moving from frozen gas hydrate bearing sediment above the GHSZ into free gas or water bearing

sediment below (Kvenvolden & Lorenson, 2001). The presence of free gas at the hydrate phase boundary is believed to be the principal control on the amplitude of the observed BSR (Holbrook et al., 1996). Blanking can be used as a qualitative indicator of increased hydrate concentration in some cases of strata with uniform lithology displaying lateral seismic reflection amplitude contrasts above the BSR (Hornbach et al., 2003).

Figure 4.2:(a) Seismic transect A-A' from Blake Ridge (see Fig. 1a) with key features visible such as erosional scouring of seabed; sediment waves and characteristic gas hydrate related BSR. Some studies have noted the existence of scattered, deeper bright spots occurring below the BSR, which are surmised to be gas pockets (Hornbach et al., 2003). (b) Schematic view seismic transect of A-A' from Blake Ridge adapted from (Hornbach et al., 2008).

4.2.3 Discrepancies in GHSZ

A key source of debate following ODP Leg 164 site investigations has been the discrepancies between the observed base of GHSZ and thermodynamic base of GHSZ as predicted from phase relationships. ODP Sites 955 and 997 display BSR at depths (~ 440 mbsf) (Fig. 4.3a) far

above the estimated thermodynamic depth for the base GHSZ (~520 mbsf). One hypothesis explaining these inconsistencies is detailed below.

The deposition in this area is dominated by hemipelagic accumulations of biogenic and terrigenous sediment that is modified and reworked by contour currents associated with the WBUC (Paull et al., 1996a). High velocity (40 cm s^{-1}) WBUC erodes into the sediments of the Blake Ridge, which in turn will lead to the re-equilibration of the GHSZ in response (Hornbach et al., 2003). In principle the BSR is thus forced downwards due to the cooling of previously gas charged zones that were in the free gas domain now falling within the envelope for hydrate formation. As a result, reflectors bearing the hallmarks of hydrate related BSRs such as opposite seismic polarity to the seabed can be found at depths well within the accepted GHSZ. These have variously been referred to as palaeo-BSRs in the literature.

The indicators for the existence of a hydrate and free gas multi-phase model arose from discrepancies between previously modelled predictions of hydrate concentrations and the results of chemical profiles (Burwicz & Rüpke, 2019). Estimates of hydrate concentration vary between 2 – 7% (Egeberg & Dickens, 1999; Paull et al., 1996a; Wood & Ruppel, 2000). The multi-phase component simply proposes the existence of both frozen hydrate and free gas together at the GHSZ (Paganoni et al., 2018).

Figure 4.3: (a) 2D seismic reflection profile displaying relative positions of ODP Sites with BSR position marked in red (dashed line is extrapolation of BSR not observed at Site 994 based on trend). High amplitude reflectors corresponding to free gas charged sediments are observed below clear BSR in Sites 995 and 997. Panels overlain with ODP data for sonic log (b), VSP (c) and borehole temperature measurements (d). Note the sharp drop in recorded velocities below the BSR at Site 995 and 997 for VSP. Adapted from (Holbrook, 2001; Paull & Matsumoto, 2000)

4.3 Materials and Methods

The subsurface thermal modelling workflow is underpinned by the use of seismic data. A key component of the workflow is the presence of an identifiable BSR on seismic reflection data to help derive a proxy for shallow heat flow. This workflow has been applied in this area with some modifications (Fig. 4.4) through the use of one-dimensional models of subsurface temperature corresponding to existing ODP sites.

Figure 4.4: Workflow utilised in this study for estimating subsurface temperature.

4.3.1 Shallow thermal regime

Previous literature has demonstrated the use of mapping BSRs at the base of gas hydrate stability to mark an isotherm (Calvès et al., 2010; Serié et al., 2017; Vargas-Cordero et al., 2010). Hydrate stability is primarily controlled by pressure and temperature, and to a lesser extent other factors

such as salinity of the pore fluid or the composition of trapped gases (Dickens & Quinby-Hunt, 1994; Sloan et al., 1998). Gas hydrates in the Blake Ridge have been extensively studied and as such their geochemical parameters are well constrained (Egeberg & Dickens, 1999). By identifying the BSR on seismic reflection data, assuming that it marks the base of the GHSZ, application of a suitable hydrate stability phase model can enable the derivation of temperature at this depth. The seismic reflection volume is in the time domain, thus depth conversion of the two-way travel time (TWT) seismic horizons must be completed. This is to determine both temperature and pressure conditions at the sediment water interface and the phase boundary. Extensive velocity analyses of the Blake Ridge subsurface have revealed that the seabed velocities are low ($\sim 1400 \text{ m s}^{-1}$) and these low velocities are likely not artefacts (Hornbach et al., 2003). A constant velocity (of 1480 m s^{-1}) has been utilized for the depth conversion of the seabed. In the absence of a detailed velocity model, vertical seismic profiler (VSP) velocities (Fig. 4.3c) from the nearby ODP sites are averaged over the interval depths corresponding to the recorded GHSZ. This is done in order to maintain consistency with the use of these velocities at a later stage to derive thermal conductivity variability with depth. An isopach map in TWT of the GHSZ thickness is created. Using the interval velocity averaged over the GHSZ (1688 m s^{-1}), the isopach map is converted to represent a depth thickness to which the seabed depth for each point in XY coordinate space are convolved. In doing so a BSR depth map is produced, which combined with our seabed depth map are the two primary deliverables from seismic interpretation that are necessary for the subsequent thermal regime modelling.

As stated earlier the conditions for hydrate stability must be defined. Key parameters include the trapped gas composition and fluid salinity. Most of the recovered cores from Sites 994, 995 & 997 are noted as being gassy, with reports noting significant degassing of some sections (Paull et al.,

1996b). The released gas is mostly methane with minor quantities of CO₂. This is supported by gas samples taken from piston core samples which show a primarily methane hydrate with up to 98% methane, ~1% CO₂ and negligible amounts of ethane and propane from total volumes exceeding 350 mL (Paull et al., 1996b,c). Chemical analyses of water samples from pressure core samplers (PCS) at Site 995 for example yield an average salinity of 33.3 g kg⁻¹ (Paull et al., 1996c). Interstitial water chemistry yields an identical average salinity, consistent with the assumption made for modelling. Site 997 also has very similar interstitial water chemistry to Sites 994 and 995 (Paull et al., 1996d). A later ODP Leg 172 targeting the nearby area also recorded salinity records consistent to an average salinity of 33.3 g kg⁻¹ (Keigwin et al., 1998).

With trapped gas composition and fluid salinity established, a suitable model for the hydrate stability field must be utilized. Two such models are utilized, based on the experimental work of Dickens & Quinby-Hunt (1994); and Lu & Sultan (2008), referred to as Model 1 and Model 2 respectively. Dickens & Quinby-Hunt's hydrate stability relationship (Equation 1) is adapted for temperature at the phase boundary (Dickens & Quinby-Hunt, 1994).

Equation 1:
$$T_{BSR} = ((3.79 \times 10^{-3} - 2.83 \times 10^{-4}(\log(\rho \times g \times Z_{BSR})))^{-1}) - 273$$

Where T_{BSR} is the temperature at GHSZ (°C); ρ is density (kg m⁻³) (of seawater); g is acceleration due to gravity (m s⁻²) and Z_{BSR} is the depth (m) of the BSR.

Similarly Lu & Sultan's relationship (Equation 2) is adapted to give temperature at the phase boundary in degree Celsius instead of Kelvin as in the original equation (Lu & Sultan, 2008).

Equation 2:
$$T_{BSR} = \frac{(\ln P - \ln F_s - E_s S)}{C_s S + D_s} - 273$$

Where T_{BSR} is temperature at the BSR (°C); P is pore fluid pressure (MPa); S is salinity; F_s , C_s , D_s & E_s are empirical constants.

$$F_s = 1.010769956 * 10^{-9}; C_s = 0.1711726397; D_s = 0.1046133676; E_s = -34.14836102$$

Both hydrate stability modelling scenarios are made assuming pure methane as the trapped gas and seawater as the interstitial fluid with a salinity of 3.35%. A hydrostatic fluid pressure gradient is also assumed for the modelling scenarios. Water density ρ_w of 1054.6 kg m⁻³ is based on pressure data from ODP records, and is consistent with density expected for deep water in the North Atlantic (Wang et al., 2010). ODP records also indicate that pore pressures, particularly at the crest of the ridge were marginally (up to 0.000526 MPa m⁻¹) above hydrostatic pressure (Paull et al., 1996d). Fluid overpressure is to be expected near the crest of the ridge, as fluids can be expected to migrate up from the flanks, which are expected to be under-pressured. The degree of overpressure increases from Site 994 to Site 997 in accordance with the increasing proximity to the ridge crest (Paull et al., 1996b, 1996c, 1996d). Studies of the elastic properties of uncompacted and overpressured sediments show that for this degree of fluid overpressure, acoustic velocities will increase by a negligible amount (~2 – 4 %) (Lee, 2003). Furthermore ODP thermal conductivity data was corrected to seafloor temperature and hydrostatic pressure conditions (Ratcliffe, 1960). Having the BSR mapped in the depth domain enables the calculation of hydrostatic pressure at this depth.

Bottom water temperature (BWT) or the temperature at the sediment water interface (SWIT) can be acquired from open source literature such as the National Oceanic and Atmospheric Administration (NOAA) World Ocean Atlas (WOA) (Boyer et al., 2005; Locarnini et al., 2013). These are annualised mean data points for water column temperatures at standard depth intervals as defined by NOAA. The resolution of this data is either at 0.25° or 1° grid spacing. It must be noted that during the 1D modelling of pseudo boreholes corresponding to existing ODP sites 994, 995 and 997, the WOA temperature record from the nearest geographic grid node did not extend

deep enough to the seabed in these locations. Instead the authors utilized a means of interpolating seabed temperature by synthetically modelling the hydrothermal gradient. This assigns simple regression fit to raw WOA data corresponding to three main pelagic subdivisions of the water column (Sarkar & Huuse, 2021b).

Equation 3:
$$T_{SEABED} = (0.0001 * Z^2) - 0.038 * Z + 22.923 \quad \text{if } Z \leq 200$$

$$T_{SEABED} = (0.00000003 * Z^3) - (0.00007 * Z^2) + 0.0318 * Z + 14.863$$

$$\quad \text{if } 200 < Z < 1000$$

$$T_{SEABED} = 1423.4 * Z^{-0.791} \quad \text{if } Z \geq 1000$$

where T_{SEABED} is the modelled hydrothermal gradient temperature (°C) and Z is seabed depth (m). If temperature at seabed is known, a simple linear geothermal gradient can be established using the following relationship.

Equation 4:
$$\frac{dT}{dZ} GHSZ = \frac{T_{BSR} - T_{SEABED}}{Z_{BSR} - Z_{SEABED}}$$

Where dT/dZ is geothermal gradient (°C km⁻¹); T_{BSR} is temperature at BSR (°C); T_{SEABED} is seabed temperature (°C); Z_{BSR} is depth of BSR (km); Z_{SEABED} is seafloor depth (km).

4.3.2 1D modelling of boreholes

The BSR derived shallow geothermal gradient may be compared to published geothermal gradients in the ODP record. Basin modellers may choose to use this derived geothermal gradient to extrapolate temperature in the subsurface across the area of interest and also use it within 1D or 2D models. For this study, the nearby ODP boreholes will form the basis for 1D models corresponding to each site. Creating these models is necessary as the borehole locations lie outside the extent of the 3D seismic reflection data (Fig. 4.1b). To model the thermal profile for each borehole, further information about the subsurface thermal regime such as thermal

conductivity and heat flow are needed. If we assume a constant thermal conductivity over a range of depths with corresponding temperature measurements, and that heat transfer is solely vertical and occurs through conduction only, it becomes possible to calculate heat flow using the 1D approximation of Fourier's Law as shown in Equation 5.

Equation 5: $Q = k \times \frac{dT}{dZ}$

Where Q is heat flow (mW m^{-2}); k is thermal conductivity ($\text{W m}^{-1} \text{K}^{-1}$) and dT/dZ is geothermal gradient ($^{\circ}\text{C km}^{-1}$).

Heat flow probe data is rare and published heat flow information is usually derived from boreholes using thermal conductivity and geothermal gradient. Thermal conductivity is a measure of how well heat is conducted through a material (Popov et al., 2003). Thermal conductivity probe data is difficult to gather, suffering from contact issues between the measurement tool and borehole wall (Brigaud et al., 1990; Nole et al., 2017). There has been extensive study into deriving thermal conductivity from other physical parameters such as velocity measurements for example (Esteban et al., 2015; Leadholm et al., 1985; Pimienta et al., 2018; Rosenbaum et al., 2007). Thermal conductivity is found to be sensitive to mineral composition, porosity and the presence of fractures (Gegenhuber & Schoen, 2012; Hartmann et al., 2005). Velocity is also sensitive to these factors. An empirical transformation from velocity to thermal conductivity has been developed (Equation 6) and adapted from existing experimental data for samples covering a wide array of major lithologies. Best fit regressions have been applied through sample points for wet sample points only, in order to best represent the fluid saturation in the subsurface of the study area (Fig. 4.5). In previous work (Sarkar & Huuse, 2021b) acoustic velocity in the form of seismic processing velocities were used in Equation 6 to derive thermal conductivity. Due to the lack of

such seismic processing velocities in this area, borehole velocities from VSP data have been utilized (Fig. 4.5).

Equation 6: $k_V = 2.1409 \ln V_p - 14.759$

Where k_V is thermal conductivity from velocity ($\text{W m}^{-1} \text{K}^{-1}$) and V_p is P wave velocity (m s^{-1}).

Figure 4.5: Empirical velocity to thermal conductivity transform utilized in this study. Data shown includes published experimental data for wet samples. Adapted from Boulanour et al. (2013); Grevemeyer & Villinger (2001); Hartmann et al. (2005); Jorand et al. (2015); Leadholm et al. (1985). In previous work (Sarkar & Huuse, 2021b) additional data points were utilised for this empirical transformation containing data from studies such as Mielke et al. (2017). These contained sample data for igneous lithologies for example. Lithological constraint for the target interval for the Blake Ridge is absent such lithologies. Thus, some of those previously used studies were excluded from the point cloud, with the belief that a better fit for the thermal conductivity of the shallow sediments of the Blake Ridge would be determined.

The shallow geothermal gradient valid for the GHSZ (Equation 4) can be used alongside the derived thermal conductivity (Equation 6) to derive a shallow heat flow proxy for each borehole

(using Equation 5). To compute such a heat flow proxy valid for the GHSZ, thermal conductivity in each 1D borehole model is averaged over the GHSZ interval. Calculating such a BSR heat flow proxy has its advantages. A BSR heat flow proxy corresponds to BSR extent on seismic data as opposed to traditional point measurements (Shankar et al., 2014). At this stage each borehole model has an existing synthetic thermal conductivity profile (derived using Equation 6).

Temperature below seafloor is a function of depth below the seafloor and the geothermal gradient. Instead of extrapolating the shallow geothermal gradient valid only for the GHSZ, it is possible to use the BSR heat flow proxy and derived thermal conductivity to compute a nonlinear geothermal gradient. It is now possible to use this geothermal gradient to calculate temperature at any given point below the seabed (Equation 7), with the addition of seabed temperature necessary to incorporate the impact of the hydrothermal gradient on the temperature of shallow sediments.

Equation 7:
$$T = T_{SEABED} + \left(\frac{dT}{dZ} \times Z_{SUBSURFACE} \right)$$

where T is predicted temperature (°C); T_{SEABED} is the temperature at seabed (°C) (Equation 4); dT/dZ is the instantaneous geothermal gradient (°C km⁻¹) (Equation 5); and $Z_{SUBSURFACE}$ is the subsurface depth (km).

A seismic interpretation suite (Schlumberger Petrel) was used for the seismic interpretation and shallow thermal regime modelling in 3D (Cox et al., 2020; Posamentier, 2004). The 1D models were compiled on spreadsheet software (Microsoft Excel).

4.4 Data

The data for this project is entirely open source and can be subdivided into two distinct types, seismic data and borehole data. The seismic data is used primarily for the estimation of a shallow

geothermal gradient and shallow heat flow proxy derived from the BSR. In the absence of seismic velocities, the borehole data acts not only as calibration for the test results but provides a proxy for velocity data.

4.4.1 Borehole data

Borehole data formed the primary data for this study. The ODP Sites 994, 995 & 997 from Leg 164 investigating the Blake Ridge Hydrate province were chosen (Fig. 4.1b), particularly due to their proximity (within 10 km) to the available 3D seismic survey (Hornbach et al., 2008; Wood & Ruppel, 2000). The full suite of physical data logs was available from these sites, of which VSP (Fig. 4.5a), thermal conductivity (Fig. 4.5b) and borehole (in situ-) temperature (Fig. 4.5c) recordings were of most interest in this study. These measurements extend to hundreds of meters below the seafloor, thus making it suitable as calibration points for the estimation (Fig. 4.7).

Both zero offset (ZO) and walkaway (W-) VSP measurements were made using a three component Woods Hole Oceanographic Institution (WHOI) borehole seismometer by the *Cape Hatteras* (Paull et al., 1996b). ZO VSP data was available for all three sites whereas W-VSP was available for Sites 994 and 995 only. ZO VSP was taken at 8 to 10 m intervals returning ~85 traces while W-VSP interval spacing in the hole was ~72 m (Paull et al., 1996a) .

Primarily the ZO VSP helps ascertain free gas presence from the velocity changes below the GHSZ as the down going waves yield the most accurate P-wave interval velocities (Paull et al., 1996a). W-VSP in turn allows the examination of lateral changes in acoustic structure due to the ability to generate both P-waves and converted S-waves, which in turn informs the hydrate development model (Paull et al., 1996a).

ODP in situ temperature measurements are made using a combination of instruments. The two primary instruments used are the Adara and the water-sampling temperature probe (WSTP). A further tool used at the time was the then prototype Davis-Villinger Temperature Probe (DVTP). These tools are each used in slightly differing circumstances. The Adara APC temperature shoe is used in combination with advanced piston coring (APC) above depths of 170 mbsf. The WSTP and DVTP can be used with an extended core barrel (XCB) and tends to be used for deeper readings. The Adara tool is considered the most reliable in terms of the temperature measurements both due to the greater stability of the data logger and since the readings are calculated from an average of four data records made during firm penetration of the APC tool through hydraulic firing into the sediments (Paull et al., 1996). Measurements made by these other tools require significant corrections to match BWT recorded by the Adara tools (Paull et al., 1996c). When correcting in situ temperature recordings to equilibrium temperature, a shift of $\sim 0.3^{\circ}\text{C}$ is necessary to account for the discrepancy with the temperature at the mudline. Though statistically only 43% of ODP sites between Legs 101 – 180 with sediment temperature records had reliable temperature measurements, the in situ temperature data at Blake Ridge have been filtered for any erroneous data in order to best calibrate the estimated temperature profiles (Pribnow et al., 2000). Additional thermal data is available from the global heat flow compilation by the International Heat Flow Database (see 4.10 Appendix) (Gosnold & Panda, 2002).

Figure 4.6: Available data from ODP Leg 164 Sites 994, 995 and 997 plotted for comparison against each other; (a) Velocity data (b) Thermal conductivity measurements; (c) In situ temperature recordings. BSR depth marked on the basis of average GHSZ thickness across all three sites (see Table 4.1)

4.4.2 Seismic data

This study uses 3D multi-channel, post-stack, time-migrated seismic reflection data from offshore South Carolina (Hornbach et al., 2018). It was acquired to image multiple subsurface geological features (Fig. 4.2) including the BSR observed at the ridge crest and the more complex geology on the eastern flank. The survey also targeted part of the eroded sediment wavefield as well as the south east crest of the Blake Ridge itself (Hornbach et al., 2008).

The 3D seismic survey covers an area of 348.93 km² and was acquired by the Lamont-Doherty Earth Observatory *R/V Maurice Ewing* in 2000. It is a 40-fold survey with a 2 ms TWT sample rate and grid spacing of 75 m and 37.5 m for inline and crossline respectively. The data was stacked, band pass filtered between 20 to 160 Hz and migrated at a constant velocity (Hornbach et al., 2003). This migration velocity was taken as 1500 m s⁻¹.

Table 4.1: Combined borehole model input and output table. Thermal modelling input parameters derived from reported ODP Leg 164 data (Paull & Matsumoto, 2000). Geothermal gradient as reported has been calculated over the depth interval corresponding to the GHSZ in each borehole. Heat flow data is from the International Heat Flow Commission (see Appendix 4.10, Table 4.2) (Gosnold & Panda, 2002). Output results for each borehole are from 1D modelling. Seabed and BSR depth from depth conversion of 3D seismic pick. Temperature at mudline and BSR computed using the seismic pick based depths. For Site 994 thickness is based on extrapolated BSR depth on published 2D seismic reflection lines. Interval velocities V_{INT} are from reported ZO VSP data for corresponding borehole. Thermal conductivity K_v derived using Equation 6. Average thermal conductivity across all 3 boreholes used to map lateral heat flow variability at BSR depth on seismic as displayed in Fig. 4.7e.

Model	Parameter	Unit	994	995	997	AVERAGE
INPUT	Seabed	m	2799.1	2778.5	2770.1	
	GHSZ thickness	m	429	440	464	444.3333
	ρ_{water}	kg m ⁻³	1049.1	1055.9	1058.8	1054.6
	P gradient	MPa m ⁻¹	0.0106	0.0102	0.00999	0.0103
	Salinity	%	3.35	3.35	3.35	
	Velocity (averaged over GHSZ)	m s ⁻¹	1654	1696	1710	1686.67
	Trapped gas		Methane	Methane	Methane	
	Temperature at BSR	°C	n/a	18.7	20	
	Mudline temperature	°C	3.1	3	2.7	
	Geothermal gradient	°C km ⁻¹	35.4	33.5 ± 0.9	36.9 ± 0.4	35.3
	Heat flow	mW m ²	35	34	36	35
OUTPUT	Seabed	m	2805.47	2782.738	2772.252	
	BSR	mbsf	433.5517	434.2092	448.6836	438.81
	Mudline temperature	°C	2.671378	2.687033	2.693476	2.68

	Temperature at BSR	°C	22.94231	22.90107	22.9019	22.92
	Thermal conductivity derived from velocity	W m⁻¹ K⁻¹	1.01	1.09	1.08	1.06
	Shallow geothermal gradient	°C km⁻¹	46.8	46.6	45	46.13
	Heat flow computed from BSR	mW m²	47.1	50.9	48.5	48.83
	Temperature prediction RMSE	°C	2.25	2.27	1.23	1.92

4.5 Results

It is important to note that ODP Sites 994 and 995 are coupled locations (Paull et al., 1996c) and help study profound differences in acoustic responses, manifesting as a BSR or lack thereof, in spite of near identical subsurface geological conditions. Other than a 20 m bathymetric difference, seismic reflection profiles reveal seafloor parallel reflectors with continuous stratigraphy at both sites.

4.5.1 Sensitivity analyses

The BSR at Blake Ridge has been extensively studied and reported. Therefore, the reported values for GHSZ thickness and BSR depth from ODP records (Table 4.1) have been used in this study to calibrate the mapped BSR using the 3D seismic volume. There is no record of a BSR at Site 994 although geochemical evidence indicates hydrate presence. Thus the depth of the BSR at this location has been estimated using the trend of the BSR in corresponding sites (Holbrook, 2001). Two primary modelling scenarios were conducted on the basis of experimentally derived hydrate stability fields. To determine which model is most suitable for use at the Blake Ridge, the estimated temperatures were compared to the in situ temperature records for each ODP site, using the same input parameters for salinity; trapped gas composition; and pressure gradient (Table 4.1). The model with the least divergence from the reported values was deemed to be the desired hydrate stability phase model to use for the workflow. Model 1 (Dickens & Quinby-Hunt, 1994) had a divergence of 18.2% (averaged between all sites) from reported in situ temperature, whereas Model 2 (Lu & Sultan, 2008) had an average divergence of 13.9%. Thus Model 2 was deemed to be best representative for the hydrate stability field. To investigate the impact of the

different modelling approaches further, the sensitivity of each modelled output was tested and compared between the two approaches. Modelled parameters are overestimated using the (Dickens & Quinby-Hunt, 1994) approach, with similar sensitivity between modelled ODP sites. Between sites, the percentage difference varies by 0.01 – 0.02% for BSR temperature, shallow geothermal gradient and BSR derived heat flow proxy. Additionally, the shallow geothermal gradient and BSR derived heat flow have the same sensitivity. This is to be expected given the direct proportionality as shown in Fourier's Law (Equation 5). The greatest variation is only for the final temperature estimation for Site 994. This may be a consequence of the along trend extrapolation method to determine an estimated position of a BSR in this location, and the fact that Site 994 had fewer than half the modelled points over which the discrepancy percentage amounts were averaged (28, 64 & 67 modelled points for Sites 994, 995 & 997 respectively).

4.5.2 Thermal modelling results contrasted: 3D & 1D modelling approaches

Modelling the thermal regime in 3D using seismic data allows lateral variability (Fig. 4.7) to be examined compared to the 1D modelling approach conducted for the ODP Sites. The depth domain converted seabed (Fig. 4.7a) was calibrated against GEBCO bathymetric data (Becker et al., 2009) at 200 m contour intervals. The domain conversion was found to be on average 1.06% shallower compared to the GEBCO bathymetry. The erosional scouring at the seabed visible in the north western quadrant (Fig. 4.7a) is in concordance with the eroded sediment wavefield noted in previous studies (Hornbach et al., 2008).

Temperatures at the seabed (SWIT) modelled using WOA data (Fig. 4.7b) are an average of 8.15% lower than mudline temperatures reported from borehole temperature measurements. The

magnitude of misfit in this input parameter for the modelling is similar to other modelled parameters (see Section 4.5.1).

BSR depth (Fig. 4.7c) ranges between 2952 – 3172 mbsf with corresponding pressures of 29.8 – 32.0 MPa of hydrostatic pressure head. Using Model 2 (Equation 2), BSR temperature modelled over 3D seismic ranges between 21.2 – 22.8 °C with an average temperature of 22.4 °C (Fig. 4.7d). The coolest regions of the BSR (Fig. 4.7d) correspond with the shallowest depth for the base of GHSZ (Fig. 4.7c) as would be expected from the hydrate stability field curve (Fig. 4.7f). Results of the 1D model are compared to the reported ODP data for Sites 995 and 997. BSR temperature is 22.9 °C for both Sites 995 and 997 using the 1D modelling approach versus 18.7 °C and 20 °C respectively from ODP records (Paull et al., 1996).

The shallow geothermal gradient computed using the BSR (Equation 3) can be compared against the results reported within the ODP report (Paull et al., 1996a, 1996b, 1996c). For Site 994 the reported geothermal gradient was 35.4 °C km⁻¹ (<320 mbsf); for Site 995 it was 33.5 ± 0.9 °C km⁻¹ (<381 mbsf); and for Site 997 it was 36.9 ± 0.4 °C km⁻¹ (<414.1 mbsf) (Table 4.1) (Paull et al., 1996a, 1996b, 1996c). From the 1D modelling the corresponding shallow geothermal gradients computed over the GHSZ (thickness reported in Table 2) are 46.8 °C km⁻¹; 46.6 °C km⁻¹; and 45.0 °C km⁻¹ for Sites 994, 995 and 997 respectively. The BSR derived geothermal gradient is on average 10.9 °C km⁻¹ higher than the value reported by the ODP though it must be noted that the ODP results are not reported over the full extent of the corresponding GHSZ and that this might result in some of the discrepancy.

The modelled heat flow ranges between 42.9 – 56.2 mW m⁻² with an average of 47.8 mW m⁻² and has been computed at the base of GHSZ to demonstrate the lateral variability within the extent of the 3D seismic reflection data (Fig. 4.7e). The pockmarked variations in heat flow laterally can

be directly attributed to variations in geothermal gradient at the same positions. The pattern of this variability corresponds with bathymetric variations resulting from features such as the erosional scouring (Fig. 4.2a). The greater seabed depth at the erosional scouring implies cooler seabed temperatures at these locations. Though BSRs mimic seafloor morphology, the rapid rate of erosion due to the WBUC would not allow the observed seismic marker, that is, the phase boundary of gas hydrates to re-equilibrate quickly enough. Thus, the BSR below the erosional scours will not be proportionately deeper and as a result the GHSZ is thinner in this location. As a consequence, the shallow geothermal gradient (Equation 4) will be higher in this region, which using Fourier's Law (Equation 5) directly translates to the higher heat flows observed. Similarly, regions of raised relief are marked by low heat flow (Fig. 4.7e) as the computed shallow geothermal gradient will be lower. Heat flow modelled at point locations during the 1D modelling (Table 4.1), although outside the extent of the 3D seismic reflection data, all lie within one standard deviation of the mean heat flow. Heat flow modelled at Site 997 is closest to the average heat flow modelled from seismic data (0.41% lower). It is possible the proximity of this site to the edge of the extent of the seismic data (Fig. 4.1a) contributes to this. On average, heat flow modelled at ODP sites are 0.51% higher than the average reported from the estimation using the BSR. Therefore, heat flow modelled at point locations or using seismic data will produce consistent results.

Figure 4.7: Subsurface seismic interpretation and thermal modelling results. (a) Seabed depth map with visible erosional scouring in NW corner. (b) Seabed temperature map with temperatures modelled from NOAA WOA data as shown from the modelled hydrothermal gradient (see (f)). (c) BSR depth map. (d) Temperature at the base of the GHSZ as defined by the hydrate stability field. (e) Shallow heat flow estimated using BSR derived shallow geothermal gradient and thermal conductivity averaged across the GHSZ. (f) Hydrate stability field modelled at ODP Site 997 for a pure methane saltwater mixture displayed with the modelled hydrothermal gradient (Dickens & Quinby-Hunt, 1994; Lu & Sultan, 2008). NOAA WOA recordings from the nearest measurement

node do not extend deep enough to reach seabed at Site 997. Thus, a synthetic hydrothermal gradient is used to extrapolate to the sediment water interface.

On average the subsurface temperature predicted using the presented methodology is found to be an average of 1.53 °C higher than the in-situ temperature readings for each site. The estimated temperature profiles closely follow the trend of the measured data. Sporadic negative temperature excursions are observed such as at ~340 mbsf at Site 997 (Fig. 4.9c). Low temperature thermal anomalies in hydrate bearing sediment can be attributed to the hydrate dissociation process, which is endothermic in nature (Sloan, 1990). Negative temperature excursions shown in the predicted temperature profiles (particularly Sites 995 and 997) are observed at depths consistent with the thermodynamic base of the GHSZ (reported to extend down to ~540 mbsf). These temperature excursions would appear to support the hypothesis of hydrate existing in a multi-phase system comprising frozen hydrate and dissociated free gas down to the thermodynamic base of the GHSZ. It must also be noted that any trends in the velocity profile can be expected to translate through the modelling workflow to the final temperature output. The excursions in the temperature signal could be an artefact of a velocity change recorded by the borehole seismometer. Equally if a lithological interface causes the velocity response, it can be expected that the contrast in thermal properties across this interface would have a corresponding temperature contrast.

Figure 4.8: (a) Existing subsurface temperature profile from ODP data for Blake Ridge; (b) Subsurface temperature profile estimated using the seismic workflow. Temperatures are calculated from the velocities not only down to the interface at the base of the GHSZ marked by the BSR, but also ~200 m below it.

Figure 4.9: Predicted temperature profiles (solid blue line) for (a) Site 994; (b) Site 995; and (c) Site 997, using the workflow discussed against the reported borehole in situ temperature recordings (orange points). BSR depth at each location is shown for reference (solid green line). 95% confidence interval bounds representing the outer limits of predicted results are also shown (dotted blue line). Error bars are based on root mean squared error (RMSE) at each site (Table 4.1). Due to VSP record not going to mudline at Sites 994 and 997, velocity readings from Site 995 were substituted. Average discrepancies in measurements are 11.5%, 16.4% and 10.8% respectively over the corresponding temperature range, with a combined average of 12.9% higher than the borehole temperature readings.

4.6 Discussion

In a predictive workflow reliant on multiple parameters, uncertainty in the final derived property can become compounded. In order to determine the range within which the predicted properties vary, they are modelled using upper and lower bounds corresponding to 95% of all values. In this manner it was possible to determine the upper and lower bound for the heat flow derived from BSR (interpreted on the 3D seismic volume). Determining this heat flow bound (using Equation 5) required the upper and lower bound for interval velocity within the GHSZ and the corresponding thermal conductivity to be known. Shallow geothermal gradient is considered unchanged as the variability in the seafloor depth and BSR depth is considered negligible, and since the composition of the hydrate in this area is well known, the temperature at BSR will not vary greatly. Heat flow ranges between $35.7 - 73.5 \text{ mW m}^{-2}$. This range is consistent with reported International Heat Flow Database results in the study area (Pribnow et al., 2000). When applying the same 95% confidence interval technique to establish a range within which the temperature predictions will lie, it becomes apparent the upper bound is considerably higher (Fig. 4.9). The lower bound roughly lies within one standard deviation of the mean case thermal profile. When tracing the sensitivity of the upper bound it is found that the regression representing thermal conductivity from velocity is the source of this great variability. Velocities in the GHSZ in this area when plotted against Fig. 4.5 would all cluster around the lowest end of the point cloud. When computing the 95% confidence interval bounds for the whole array of points, the regression will include much higher velocities and correspondingly much higher thermal conductivity as the upper bound. This is what leads to the much higher upper bound seen in Fig. 4.9. If focusing only on those experimental data points corresponding to the velocities within the GHSZ (Grevemeyer & Villinger, 2001), it is not possible to derive a statistically valid regression ($R^2 < 0.1$). Thus, it must be noted that though the range of possible temperature predictions using the regression

from Fig. 4.5 (Equation 6) is large, it still provides the best possible means of deriving a first pass approximation that fits well to recorded data. RMS error has been used as a measure of accuracy to compare forecasting errors in predicted temperature against the reported data from ODP studies (Barnston, 1992). Results from the model have an RMSE between 1.23 – 2.27 °C (Table 4.1).

A significant caveat remains the sensitivity of acoustic velocity. A direct relationship (Equation 6) has been made between velocity and thermal conductivity but such a relationship becomes compromised if velocity is independently affected by another factor. This may be the impact of fluid over-pressure on recorded velocities or it could be the impact of mineral layering within the rock column on thermal conductivity. Another assumption made is the dominance of heat transport through conduction in the area, thus enabling the use of Fourier's Law to underpin the thermal modelling work. The modelling results from the Blake Ridge dataset have not demonstrated an impact from any of the above factors, though it provides an opportunity for further investigation using a dataset that allows for the impact of these factors on the modelling workflow to be explored. A data rich basin such as the North Sea Basin would prove an excellent setting for such a study and this has been explored in Sarkar & Huuse (2021a) (see Chapter 5).

Characterising subsurface thermal regime using 3D seismic data presents an opportunity to examine the lateral variability in thermal properties not hitherto possible with point data. This is best demonstrated in Fig. 4.7e where the heat flow variability is mapped on the GHSZ interface. These lateral variations can further be tied to the topographic variability at the sediment interface, indicating the manner in which structural and bathymetric features may impact the transfer of heat in the shallow subsurface. This data can then be viewed in real time on seismic interpretation software. The scale at which the variability in heat flow can be discerned in this manner is far smaller than the magnitude larger scale of available heat flow

maps in the literature. Furthermore, with the greater extent of modern-day seismic coverage in comparison to point heat flow data, it may become possible to fill in gaps in lateral coverage. Modelling thermal regime in this manner not only extends laterally but vertically too. The 1D modelling methodology also produced subsurface thermal models. Only 53 ODP legs between Leg 101 – 180 had temperature data (Pribnow et al., 2000). 43% of this data is regarded as being reliable. While it is not known how many of these sites also encountered gas hydrates, the standard logging suite of ODP data should be available for these. The 1D modelling approach utilised this ODP data. For continental margin ODP sites that display either geophysical or geochemical indications of gas hydrate presence, the methodology presented in this paper introduces a process for deriving reliable subsurface thermal data for such sites with extensive seismic data coverage that may lack published thermal data. Crucially, these temperature models extend the understanding of the thermal regime a further 260 – 330 m beyond existing data ODP thermal data. This would provide a means to expand the global database for subsurface thermal data, with the ancillary benefits to understanding in different domains that would be a natural corollary.

4.7 Conclusions

This study shows the results of a thermal regime characterisation methodology underpinned by seismic data from the Blake Ridge offshore east coast USA. It was able to take open source 3D seismic data to map a BSR and derive lateral heat flow variability across the crest of the ridge structure, and image the impact of erosional scouring on the seabed on heat flow in the shallow subsurface. The methodology was also able to extend the subsurface temperature record beyond the record available from nearby ODP boreholes, though it must be noted that these are predicted temperatures. This predicted thermal profile now extended through the base of hydrate stability and into the underlying gas charged sediment. Calibrating the

temperature predicted in this manner against ODP records determines that reliable first pass estimates can be derived in deep water passive margin settings where seismic data is available, but borehole data is lacking. This would be a powerful tool for geoscientists to not only further their understanding of subsurface petroleum systems but can be utilised for geothermal energy applications and monitoring the impact of temperature on subsurface microbial communities. It is envisaged that this workflow may be applied to other such deep-water passive margin basins, such as the Lüderitz Basin, offshore Namibia.

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4.10 Appendix

Table 4.2: Summarised thermal regime data points from the International Heat Flow Database along transect corresponding to ODP Sites 994, 995 and 997 (see Fig. 4.1) (Pribnow et al., 2000). Thermal conductivity measurements are made using the transient line source needle probe (Ruppel et al., 1995).

Identifier	Z	#	T	GT	#	k	k	HF	REF	Notes
		readings		G	readings					
41306	31	6		68	5		1.0	72	Ruppel et al.,	Ocean
	85						6		1995	
41307	31	7		50	7		1.0	53	Ruppel et al.,	Ocean
	30						5		1995	
41308	30	7		47	7		1.0	48	Ruppel et al.,	Ocean
	49						4		1995	
41309	29	7		44	7		1.1	50	Ruppel et al.,	Ocean
	95						5		1995	
41310	29	7		40	7		1.0	41	Ruppel et al.,	Ocean
	50						3		1995	
41311	29	7		40	7		1.0	43	Ruppel et al.,	Ocean
	15						7		1995	
41312	28	7		48	0		1.0	51	Ruppel et al.,	Ocean
	80						7		1995	
41313	28	7		43	0		1.0	46	Ruppel et al.,	Ocean
	42						7		1995	
41314	28	7		46	0		1.0	47	Ruppel et al.,	Ocean
	11						3		1995	

41315	27	7	40	7	1.0	41	Ruppel et al., Ocean
	83				3		1995
41316	27	7	43	7	1	43	Ruppel et al., Ocean
	75						1995
41317	27	7	46	7	1.0	46	Ruppel et al., Ocean
	65				1		1995
L164-997	0	0	0	0	0	36	Pribnow et al., Deep sea borehole 2000
41318	27	7	48	7	0.9	46	Ruppel et al., Ocean
	67				7		1995
41319	27	6	51	0	1.0	54	Ruppel et al., Ocean
	60				7		1995
41320	27	6	47	7	1.1	55	Ruppel et al., Ocean
	60				8		1995
L164-995	0	0	0	0	0	34	Pribnow et al., Deep sea borehole 2000
41321	27	7	46	0	1.0	50	Ruppel et al., Ocean
	90				9		1995
41322	27	7	48	7	1	48	Ruppel et al., Ocean
	83						1995
L164-994	0	0	0	0	0	35	Pribnow et al., Deep sea borehole 2000

41323	27	7	47	7	1.0	49	Ruppel et al., Ocean
	89				4		1995
41324	28	7	46	7	1.0	50	Ruppel et al., Ocean
	09				7		1995
41325	28	7	53	7	1.0	53	Ruppel et al., Ocean
	41				7		1995
AVERAGES			47.		1.0	47.434	
			05		55	78	

5. Subsurface temperature of the northern North Sea Basin

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5.1 Abstract

The North Viking Graben (NVG) is part of the mature North Sea Basin. It has been extensively drilled over many decades as a prolific hydrocarbon basin and is thus very well understood. As such it serves as an excellent setting to demonstrate the efficacy of a proprietary seismic data led approach to modelling subsurface temperatures using a state-of-the-art full waveform inversion velocity model covering the entire North Viking Graben. In a forward modelling problem, an empirical velocity to thermal conductivity transform is used in conjunction with predefined heat flow to predict subsurface temperature. The predefined heat flow parameters are set based on the range of values seen from previous studies in the area. Abundant well data with bottom hole temperature records provide calibration of results. In the inverse modelling problem, bottom hole temperatures as well as the velocity derived thermal conductivity are used to solve a 1D steady state approximation of Fourier's Law for heat flow. In this way heat flow is interpolated over the 12000 km² model area at a km scale

resolution, highlighting lateral variability in comparison to the traditional point-based heat flow datasets. This heat flow is used to condition a final iterative loop of forward modelling to produce a temperature model that is best representative of subsurface temperature. Calibration against 139 wells indicate that the predicted temperatures are on average only 0.6 °C warmer than the recorded values, with a root mean squared error range of 5 °C. Bottom hole temperature (BHT) for the recently completed Northern Lights Carbon Capture and Sequestration (CCS) well 31/5-7 (Eos) has also been modelled to 97 °C. This serves to highlight the applicability of this workflow not only towards enhancing petroleum systems modelling work but also for use in the energy transition or fundamental scientific purposes.

Keywords:

Seismic; velocity modelling; subsurface temperature

Acronyms

- BCU – Base Cretaceous Unconformity
- BHT – Bottom Hole Temperature
- BSR – Bottom Simulating Reflector
- CCS – Carbon Capture and Sequestration
- CMP – Common Mid Point
- EOR – Enhanced Oil Recovery
- FWI – Full Waveform Inversion
- GEBCO – General Bathymetric Chart of Oceans
- IDW – Inverse Distance Weighting
- MBSF – Metres Below Sea Floor
- MD – Measured Depth
- MSL – Mean Sea Level
- NCS – Norwegian Continental Shelf

- NOAA – National Oceanic and Atmospheric Administration
- NPD – Norwegian Petroleum Directorate
- NVG – North Viking Graben
- PSDM – Post Stack Depth Migrated
- PSTM – Post Stack Time Migrated
- RMO – Residual Move Out
- RMS – Root Mean Squared
- RMSE – Root Mean Squared Error
- TOMOT – Time Tomographic inversion
- Tpred – Predicted Temperature
- TVD – Total Vertical Depth
- TWT – Two Way Travel Time
- UKCS – UK Continental Shelf
- WOA – World Ocean Atlas

5.2 Introduction

The importance of understanding the subsurface temperature conditions is manifold. An understanding of the isotherms may help delineate important temperature driven diagenetic boundaries (Bjørlykke et al., 1989). Similarly, it is useful for petroleum exploration as it can instruct as to the nature of the hydrocarbons to be expected from a source rock (Allen & Allen, 2013). Unlike frontier areas where the effectiveness of source rocks may be in doubt, this is not a concern in the North Sea. However, understanding of the present-day subsurface temperature can still prove useful in such a mature basin. Analysis of global hydrocarbon resources has shown that there exists a narrow thermal window, the so called “Golden Zone” (Nadeau, 2011), where diagenetic processes for clay minerals for example are conducive to

porous reservoirs. Similarly, an improved understanding of subsurface temperature could assist in enhanced oil recovery (EOR) such as when CO₂ saturation is used to aid recovery of heavy oils by reducing the density of the latter (Davarpanah & Mirshekari, 2020). Investigations into geothermal energy also benefit from improved understanding of subsurface temperature conditions (Bonté et al., 2012; Fuchs & Balling, 2016). The North Sea is one of the world's most prolific and extensively studied petroleum provinces (Cornford, 1998; Evans, 2003; Leadholm et al., 1985; Rüpke et al., 2008). Over the course of the past sixty years numerous oil and gas fields have been discovered, many of which have served as the testing ground for new technologies such as time lapse 4D seismic or enhanced oil recovery (Awan et al., 2006; Landrø et al., 1999). With this history of developing and applying cutting edge methodologies, it is a fitting setting to test the workflow proposed here. This paper proposes and tests a means of utilising seismic data to predict subsurface temperatures. Previous work has demonstrated that a transform based on empirical velocity and thermal conductivity data may be utilised to convert seismic velocities to thermal conductivities (Sarkar & Huuse, 2021a, 2021b). The derived thermal conductivities may be used in conjunction with heat flow data, either from existing open source data or through modelling of heat flow, to determine subsurface temperatures from Fourier's Law under a steady state condition. Historically there have been numerous studies of the thermal conductivities and heat flow of sediments in the northern North Sea (Andrews-Speed et al., 1984; Brigaud et al., 1992; Cornelius, 1975; Evans, 1977; Evans & Coleman, 1974; Houbolt & Wells, 1980; Leadholm et al., 1985). However, there seems to be a hiatus in such studies in recent times. As such it is envisioned that the output from the thermal modelling work in this study will add to the existing body of knowledge in that regard.

The Northern Lights project is an initiative by the Norwegian government with industry partners to undertake full scale carbon capture and sequestration (CCS) (Cozier, 2019). The

injection well 31/5-7 (Eos) appraised the target site in March 2020 and its temperature has been modelled here to demonstrate the efficacy of the proposed methodology.

5.2.1 Thermal modelling fundamentals

To understand how subsurface temperature might be modelled in the present day it is important to establish the key thermal boundary conditions and properties. These are heat flow, seabed temperature, thermal conductivity, the resultant geothermal gradient and subsurface temperature. The link between heat flow, thermal conductivity and geotherm can be represented by the 1D approximation of Fourier's Law (Eq. 1).

Equation 1: $Q = k \times \frac{dT}{dZ}$

Where Q is heat flow (mW m^{-2}); k is thermal conductivity ($\text{W m}^{-1} \text{K}^{-1}$) and dT/dZ is geothermal gradient ($^{\circ}\text{C km}^{-1}$).

To estimate the temperature below a certain depth in the subsurface, the rate of change of temperature with depth, i.e. the geothermal gradient is the most important parameter. It becomes apparent then that by rearranging Eq. 1, the input parameters necessary to estimate this are heat flow and thermal conductivity.

Equation 2: $\frac{dT}{dZ} = \frac{Q}{k}$

Thermal conductivity is a measure of the ease with which heat may be conducted through a material (Popov et al., 2003) and is thus critical to estimating the thermal structure of the subsurface. Thermal conductivity data from direct measurements are made either in situ through well logs or via direct measurements on recovered samples (Andrews-Speed et al., 1984; Jorand et al., 2015; Schön, 2015). Measuring tools include either a needle probe inserted into a sample or a divided bar apparatus (Evans, 1977; Horai, 1982). However, these measurements may suffer from issues that affect both their ease of acquisition and reliability.

For example thermal conductivity probes may have poor contact with borehole walls, or the needle probe reading might be affected by the alignment of the mineral fabric in relation to the needle orientation (Lucazeau et al., 2004; Pribnow et al., 2000). As a result there has been considerable thought put towards deriving thermal conductivity from other more easily measured physical properties such as bulk density, porosity or compressional sound wave velocity (Boulanouar et al., 2013; Esteban et al., 2015; Gu et al., 2017; Hartmann et al., 2005; Horai, 1982; Jorand et al., 2015). In the case of velocity, it is found to have similar sensitivity to properties as thermal conductivity (Houbolt & Wells, 1980). That is, thermal conductivity is primarily affected by the mineral composition, porosity and presence of fractures (Mielke et al., 2017; Pimienta et al., 2018; Zamora et al., 1993). Temperature and pressure also impact thermal conductivity though not as much as the other factors (Leadholm et al., 1985).

Figure 5.1: Study area in the northern North Sea outlining the extent of the CGG North Viking Graben survey offshore the Norwegian continental shelf. Some key fields in the study area are named for reference. Thermal model area displayed in red. Transect A-A' based on North Viking Graben type section shown in Millennium Atlas (Copestake et al., 2003). Hydrocarbon wells displayed are used for calibration. Northern Lights CCS test well 31/5-7 also displayed (red circle) (between Brage and Troll fields). Bathymetry from GEBCO ("The GEBCO_2019 Grid - a continuous terrain model of the global oceans and land," 2019).

5.3 Geological history

The North Viking Graben (Fig. 5.2) is located in the Northern North Sea between the UK continental shelf (UKCS) to the West and the Norwegian coast to the east, and part of the north western European cratonic block (Brigaud et al., 1992). It is part of the North Sea Graben system, which controlled Cretaceous-Cenozoic subsidence of the basin (Cornford, 1998). It is a Mesozoic rift system, with the rifting in this area having occurred after the Caledonian orogeny (and extensional orogenic collapse), with there being two primary phases of extensional rifting since the Devonian (Fichler et al., 2011; Rüpke et al., 2008; Ziegler, 1992). Primary rifting in the Permian to Early Triassic was followed by a post rift subsidence period (Nøttvedt et al., 1995). The next phase of rifting was from lower to mid Jurassic to early Cretaceous and was also followed by a post rift subsidence period. The rift axis for the Permo-Triassic rifting is believed to be located under the present Horda Platform with the late Jurassic rift axis below the present day Viking Graben (Christiansson et al., 2000). No major tectonic activity is believed to have occurred post Jurassic though there is some conjecture regarding a Tertiary rifting episode (Rüpke et al., 2008) and mid Miocene inversion (Løseth et al., 2016). The predominant rift direction in the N to NE striking Viking Graben was west-east and northwest-southeast.

Crustal basement rocks in this area have a history exceeding one Wilson cycle and trace back to the junction between the Laurentian and Baltican plates, including the opening of the Iapetus Ocean, island arc development linked to oceanic subduction and the Caledonian orogeny (Fossen et al., 2008; Meert & Torsvik, 2003). The composition of the basement rocks can be seen to vary from granites underneath the East Shetland Platform to low and intermediate grade metamorphic and metamorphosed sediments below the Viking Graben and Horda Platform (Fichler et al., 2011). The sedimentary record in this area is Devonian and younger. Sand and shales dominate the Triassic to Jurassic basin fill with carbonates and shales

predominant in the Cretaceous (Brigaud et al., 1992). Tertiary lithologies consist of shales, silts and sands, with a brief period of Paleocene volcanism marked by the widespread deposition of volcanic tuffs across the graben (Haaland et al., 2000).

Source rocks in the area are predominantly Kimmeridge Clay (shales) that were deposited briefly in the Late Jurassic (Davison & Underhill, 2012; Gautier, 2005). Abundant reservoir rocks are available in the NVG (with one such reservoir including the pre rift Lower-Mid Jurassic sandstones) all of which exist with a variety of sealing mechanisms. These pre rift reservoirs are usually found in tilted fault blocks where fine-grained post rift sedimentary sequences act as seals. Commonly in the Viking Graben these vertical seals are unconformably overlying shales.

Figure 5.2: (a) East West transect (A-A' in Fig. 5.1) displaying reflection seismic data, annotated with major chronostratigraphic surfaces and structures of note. (b) Overlay of major intervals highlighting the geometry of the North Viking Graben in the west of the model area, with tilted fault blocks apparent. The study area is bounded to the west by the East Shetland Basin, with the eastern limits coinciding with the Horda platform. Adapted from Evans, 2003.

5.4 Data

The data used for the study can be subdivided into seismic data and borehole data.

The North Viking Graben megasurvey was conducted by CGG between 2014 and 2016, covering a total area of 35410 km². This broadband 3D seismic reflection survey of BroadSeis and BroadSource configuration covers the northern North Sea basin and was shot in a north-south direction, recorded in TWT down to 9 seconds with an acquisition sample interval of 2 ms (Purvis et al., 2018). It was acquired using 324 & 328 acquisition lines (due to merging of

two separate survey areas: Horda and Tampen respectively) with 6.25 x 18.75 m bin spacing and a line separation of 75 m. A (flip flop) shot point interval of 18.75 m and a source separation of 37.5 m gives a nominal common-mid-point (CMP) fold of 106. Twelve streamers were used in total, each 7950 m long, with 1000 channels towed at depths of either 6 to 9 m. Multiple algorithms were used to remove noise and multiples. Both manual picking and time tomographic inversion (TOMOT) was used to generate velocities with imaging done using Kirchhoff PSTM. A proprietary CGG methodology of continuous automatic bi-spectral velocity picking helped generate the final stacking velocities (Purvis et al., 2018). The processed PSTM and PSDM cubes underpin the modelling work conducted in this study.

The FWI technique aims to produce a high-fidelity subsurface representation of velocity, as the velocity model minimises differences between observed and modelled seismic waveforms within the original raw data (Warner et al., 2013). In making the FWI velocity product, a best guess starting model based on seismic processing velocities is iteratively improved using a sequence of linearized local inversions (Warner et al., 2013). For the CGG NVG survey the fast track velocity product was made from the Dix conversion of root mean squared (RMS) stacking velocities, followed by Kirchhoff depth migration to residual move out (RMO) velocities (CGG, 2019). By starting at low seismic frequencies with the tomography process for the FWI model build, the risk of cycle skipping was minimised (CGG, 2019). During the FWI process, the model was subdivided into smaller areas targeting regions of key geology, allowing verification to be conducted (CGG, 2019). Three production runs at ever increasing seismic frequency (4; 5.5 & 8 Hz) were conducted as part of the FWI model build (CGG, 2019). The final 8 Hz update produced the velocity model that best follows geological structure and can characterise small scale features such as injectites (CGG, 2019). The FWI model was calibrated using 101 wells with QC checks completed against sonic log data (CGG, 2019).

Borehole data for this study were primarily sourced from the Norwegian Petroleum Directorate (NPD) website. This gave access to well reports, mud logs, geological reports and wireline logging data. Because the FWI volume was already calibrated against downhole sonic velocity data and provided in the depth domain, the primary data of interest for this study were the bottom hole temperatures (BHT) recorded for each well within the thermal model area. Publicly available heat flow data from the International Heat Flow Commission database were used to provide constraint on the heat flow parameter (Gosnold & Panda, 2002). There is a scarcity of data points covering the model area as seen in Fig. 5.4 with the nearest offshore data point too distant to confidently interpolate from (Ritter et al., 2004). In the absence of suitable heat flow control a combination of published heat flow estimates from various authors has been used (Fig. 5.4) (Davies & Davies, 2010; Davies, 2013; Lucazeau, 2019).

Figure 5.3: (a) Transect displaying interval velocities from FWI velocity model, overlain with structures. With adherence to well data (well paths shown in various colours), this velocity model can be seen to show detail, corresponding with major structural and stratigraphic interfaces. Basement is marked by the transition to velocities $\geq 6000 \text{ m s}^{-1}$ (Christiansson et al., 2000; Fichler et al., 2011). (b) Transect displaying average velocities from FWI velocity model used to condition thermal model, also shown with well paths.

Figure 5.4: Existing heat flow data from the International Heat Flow Database shows a scarcity of data in the model area (Gosnold & Panda, 2002). Relying on published heat flow grids such as the Davies (2013) shown above demonstrates the coarseness of the data when compared to the scale of the model area (Davies, 2013).

5.5 Methods

The modelling work has been conducted using Schlumberger's Petrel software suite, with it being used for 3D seismic interpretation over the extent of the survey as well as to create and manipulate the property volumes and thermal models in this work. Standard seismic interpretation techniques, including horizon mapping, surface map creation and seismic attribute extractions were conducted for a structural interpretation of two reference horizons, the seafloor and the Base Cretaceous Unconformity (BCU) (Cox et al., 2020; Posamentier, 2004). The BCU follows the regional stratigraphic framework and serves as a reference

horizon, upon which model outputs are overlain as attributes, thus giving a regional context to the results (Evans, 2003). The seafloor is the ceiling for the thermal models, separating the hydrothermal and the geothermal domains. Both horizons were mapped in depth using the 3D reflection seismic data. The bathymetry was ground truthed with the open source bathymetric grid data from GEBCO (Becker et al., 2009). For the purposes of this work, no other structural interpretation was necessary. Further interpretation or import of grids can of course be done to observe the predicted temperature at desired stratigraphic levels.

The workflow utilised in this project is summarised in Fig. 5.5. It can be broken down into two main problems: the forward modelling problem uses the seismic velocity data as the input parameter to model for thermal conductivity and subsurface temperature using constant heat flows, which in turn is calibrated against available bottom-hole temperature (BHT) data; the inverse problem calculates heat flow from the observed BHTs and the average thermal conductivity volume. As heat flow is an important input parameter to model temperature, it becomes possible to update the temperature forward model with the inverse modelling results, and thus validate the final temperature model results, in a manner akin to tomographic update of velocity models (Jones, 2018; Prada et al., 2019).

Figure 5.5: Model building workflow displayed in terms of input, processing steps and outputs/deliverables. There are two main pathways, a forward modelling pathway where seismic data is used to simulate BHTs; and an inverse modelling pathway where BHTs are used to determine the heat flow conditions needed for it. This allows for an iterative final forward modelling pathway utilising the derived heat flow to arrive at a subsurface temperature model representative of present-day conditions.

5.5.1 Forward modelling problem – present day subsurface temperature

The dataset used a modern broadband seismic survey covering the North Viking Graben (NVG) spanning across parts of the UK and Norwegian continental shelves (UKCS and NCS, respectively). The full waveform inversion (FWI) final velocity model is the key seismic data product underpinning the modelling work.

5.5.1.1 Thermal conductivity structure

This study uses high-resolution 3D seismic velocity volume and experimental data relating velocity and conductivity (Fig. 5.6). By including a wide range of studies, covering a wide array of lithologies and settings, it is hoped that the resulting empirical relationship can serve as a robust first order estimate for the varying porosities encountered within the study area. The sample dataset is limited to wet samples only and measurements taken using transient measurement apparatus such as the optical scanning method (Popov et al., 1999), in order to maintain applicability to fluid filled rocks in the subsurface and parity between data points respectively. A similar approach has previously been applied in passive margin settings offshore Namibia and offshore USA (Sarkar & Huuse, 2021a, 2021b). The best fit regression through the subset of points is as follows:

Equation 3: $k_v = (6 \times 10^{-5})V_p^{1.3279}$

Where k_v is thermal conductivity from velocity ($\text{W m}^{-1} \text{K}^{-1}$) and V_p is P wave velocity (m s^{-1})

Figure 5.6: Bulk shift transform from velocity to thermal conductivity derived from experimental data published in the literature. All points displayed are wet samples with laboratory measurements of both velocity and thermal conductivity having been done with similar tools. This is to both reflect the presence of fluids in the subsurface and to also reduce the variables between displayed data respectively.

With a highly detailed FWI velocity volume representing the P-wave velocity of the subsurface and a function relating velocity and thermal conductivity, it is possible to convert the FWI velocity volume into a volume of thermal conductivity varying with depth (using Eq. 3). To facilitate the workflow the FWI interval velocity volume was first converted to an average velocity volume in depth below the seabed (as the geotherm starts at seabed) (Fig. 5.3b) and this in turn allowed the estimation of average thermal conductivity as a function of depth in the entire volume (Fig. 5.7b).

5.5.1.2 Heat flow input scenarios

In order to convert the average thermal conductivity (Eq. 2), information regarding the heat flow in the study area is required to determine the geothermal gradient. Initial heat flow

values were defined based on the nearest points in the International Heat Flow Database. As seen on Fig. 5.4, there is a paucity of data points in the study area. This leads to examining the published record for maps of heat flow covering the North Sea, and these tend to exist in the form of heat flow estimate grids at regional or global scale. Examining these grids such as Davies (2013) or Lucazeau (2019), it becomes apparent that the heat flow varies greatly. This seems to depend not just on the size of the grid squares over which the authors have applied their interpolation, but the exact technique used to interpolate and the input parameters they have used will lead to this variability. Consequently it was decided that analysis of the range of heat flow values that are observed in the literature for this area will be used to define predetermined starting conditions for heat flow (Andrews-Speed et al., 1984; Cornelius, 1975; Davies, 2013; Evans & Coleman, 1974; Harper, 1971; Leadholm et al., 1985; Lucazeau, 2019; Ritter et al., 2004). This gives a low-, mid- and high- case heat flow of 60, 70 and 80 mW m⁻² respectively.

5.5.1.3 Temperature grids & calibration

Having determined thermal conductivity and established heat flow scenarios it becomes possible to calculate three geothermal gradient scenarios for the model area. By convolving this with the subsurface depth and incorporating the bottom water temperature (BWT) (i.e. seabed temperature) an estimate of present-day subsurface temperature can be made.

Equation 4: $T = T_{SEABED} + \left(\frac{dT}{dZ} \times Z_{SUBSURFACE}\right)$

where T is predicted temperature (°C); T_{SEABED} is the temperature at seabed (°C); dT/dZ is the instantaneous geothermal gradient (°C km⁻¹) (Eq. 2); and $Z_{SUBSURFACE}$ is the subsurface depth (km).

Early studies into the geothermal aspects of the North Sea would set temperature at the seafloor to a constant, for example 10 °C (Cornelius, 1975; Evans & Coleman, 1974; Harper,

1971). Here however seafloor temperature was assigned through decadal averages from the World Ocean Atlas (WOA) dataset (Boyer et al., 2014; Locarnini et al., 2013). Using the nearest measurement node from the 0.25-degree grid of the WOA dataset, the temperature profile (hydrothermal gradient) for this was used to interpolate seafloor temperatures across the seafloor depth grid. By basing the seafloor temperatures on a decadal average, the variability of seasonal bottom water conditions and longer scale variability will be negated, thus giving a baseline temperature from which the well readings can be seen in context to, particularly with regard to determining the geothermal gradient.

Thermograms, or temperature profiles, depicting temperature change with depth are one way of displaying the model results for each well site (Cornelius, 1975). Petrel allows for the creation of synthetic logs from a reservoir model or pillar grid. This requires resampling the temperature models into a pillar grid coincident with the extent of the area of interest. Resampling of the seismic attribute volumes was done using the interpolation algorithm. The dimensions of the individual cells of the grid, and subsequently the total number of cells constituting the entire grid are important with respect to the total compute power. The modelling results displayed here have a lateral resolution of 50*50 m (XY orientation), with the top of the model coinciding with mean sea level (MSL) and the base being set at 5.5 km depth. This basal depth encompasses the maximum vertical depth of the wells used for calibration. Cell height was set to 20 m, in accordance with the vertical resolution of the velocity data. For these dimensions, the entire gridded model comprises about 1.4 billion voxels.

With all the input and derived seismic attributes resampled as properties in the pillar grid, synthetic logs for each well are generated. These synthetic logs are made for the three temperature prediction volumes coincident with the three heat flow input scenarios. The estimated temperature at the bottom of each well from the synthetic logs is then plotted

against the recorded corrected bottom hole temperature (BHT). Theoretically, the misfit between observed and modelled temperature for each well can be used to calculate how much the heat flow input for each well must be adjusted for there to be no misfit. In this way, the most representative heat flow value for the area might be calibrated.

5.5.2 Inverse modelling problem – solving for heat flow

The first stage of subsurface temperature modelling assumed 3 discrete heat flow scenarios. In this instance, discrete values for heat flow across the model area was used to simulate each temperature scenario. However, heat flow is likely not homogeneous across the model area and there may be lateral variability across individual structures and preferred fluid migration paths. If recorded temperatures in the wells are assumed to be correct and with knowledge of the seafloor temperature, geothermal gradient can be independently computed for each well site. Additionally, if the seismic velocity derived thermal conductivity is considered valid, it becomes possible to use the 1D approximation of Fourier's Law to derive heat flow at each well location. This is the inverse problem.

Equation 5:
$$Q = K_V \times \left(\frac{T_{BHT} - T_{SEAFLOOR}}{Z_{TVD}} \right)$$

Where Q is heat flow (mW m^{-2}); K_V is thermal conductivity from velocity ($\text{W m}^{-1} \text{K}^{-1}$); T_{BHT} is bottom hole temperature ($^{\circ}\text{C}$); $T_{SEAFLOOR}$ is temperature at seafloor ($^{\circ}\text{C}$); and Z_{TVD} is true vertical depth for hole bottom (km).

It must be noted that some wells are deviated and thus care must be taken not to use total depth or measured depth when computing the geothermal gradient from BHT. Instead the true vertical depth (TVD) is used with the coordinates of the hole bottom being assigned as the surface location for a pseudo well head. This is done in order to ascertain the seafloor temperature vertically above the hole bottom, thereby obviating the introduction of a lateral BWT variability element to the computation.

Interpolating for heat flow between the wells creates a map of inversely modelled laterally varying heat flow. An inverse distance weighting (IDW) function has been used to interpolate (on both ArcPro and Petrel for cross verification). The values of cells in the vicinity of the processing cell (interpolated gap) are averaged, with the distance of the neighbouring cell having an inverse weighting (Watson & Philip, 1985). Though kriging is a more advanced geostatistical procedure, it is more time consuming and thus was not pursued for this first order estimation of heat flow.

5.5.3 Final temperature model

Calibrating the results of the temperature forward model with the different heat flow input scenarios, it is likely to show different degrees of agreement. Iteratively updating the heat flow input each time and remodelling for subsurface temperature should theoretically permit the most representative heat flow across the study area to be arrived at ultimately. However, this former approach was not pursued as it was shown previously that inverse modelling allows the determination of laterally varying heat flow across the model area. Convolving this heat flow with the seismically derived thermal conductivity (Eq. 2), it should be possible to generate a volume of instantaneous geothermal gradient that has most agreement across all the calibration wells. This thermal gradient is used to generate a final temperature model (Eq. 4) that is resampled into the pillar grid and used to output synthetic temperature logs. Predicted temperature from these logs at hole bottom is extracted and used to calibrate against recorded BHT as before.

The injection well 31/5-7 is located due south west of Troll A field and targets the lower Jurassic Cook and Johanssen formations for injection. The targeted interval has ~173 m of sandstone overlain by 75 m of shale acting as a seal above it. Pressure data indicates no communication in rocks above and below the shale, reinforcing its seal properties. With no

results from this well published due to its very recent completion, it was decided to use the available details (well head coordinates and total depth) to simulate the temperature profile for this well using our model.

5.6 Results

The results from the modelling work are presented either as seismic attribute overlays on transects or by means of attribute maps on a gridded horizon. But for the purposes of calibration the primary output is the synthetic temperature log data from the wells. These results are discussed individually in the following section.

The FWI interval velocity volume was converted to an average velocity volume (Fig. 5.3), before applying the velocity to thermal conductivity transform (Fig. 5.6) to produce a volume of average thermal conductivity (Fig. 5.7b). Looking at the internal velocity derived thermal conductivity structure (Fig. 5.7a), the direct nature of the bulk shift results in the thermal conductivity variation with depth across the volume corresponding to the level of detail seen in the input velocity (Fig. 5.3). When conversion is based on the average velocities, thermal conductivity is seen to vary much more smoothly across the depth interval displayed, as expected (Fig. 5.7b). Cretaceous and younger Cenozoic sediment cover is seen to have relatively low thermal conductivities, with a distinct increase in thermal conductivity seen in the tilted fault blocks of the Viking Graben. The graben corresponds with the greatest amount of overlying sediment cover and lower conductivities relative to the neighbouring rift shoulder.

Figure 5.7: (a) Thermal conductivity from interval velocities with wells displayed. (b) Thermal conductivity from average velocities.

The forward modelling results using the predefined heat flow input scenarios are displayed on the west-east transect A-A' (see Fig. 5.8). As expected, temperatures increase gradually with depth, with no major anomalous zones seen. Cenozoic sediments are coolest with the highest temperatures in the graben itself, which makes sense considering relatively even heat flow but lower conductivities of the sediments within the graben. Isotherms are more widely spaced as we move towards the Horda Platform in the east where the conductivity is greater (Fig 5.7). Comparing the results from each heat flow scenario against each other, the broad trend is that increasing heat flow has a directly proportional effect of increasing the recorded temperature at each depth. Thus, the greatest range in the predicted temperatures is

observed in the high case heat flow model (using 80 mW m^{-2}) (Fig. 5.8c). Correspondingly the narrowest range is observed with the low case heat flow model (Fig. 5.8a). The direct impact of each heat flow input scenario is better visualised when cross plotting the temperature extracted from each well (Fig. 5.9).

Figure 5.8: Forward modelling temperature prediction profiles with transect A-A' overlain for (a) low case; (b) mid case; & (c) high case heat flow scenarios respectively. Temperature readings in the graben centre and on the graben flank are shown for reference. Highest temperatures are observed in the heart of the graben. Block like appearance is an artefact of the dimensions of the individual voxels comprising the thermal model pillar grid used to represent the subsurface.

As stated earlier, synthetic thermograms corresponding to the well path of each calibration well was extracted from the predicted temperature models. The temperature at bottom hole in each case has been plotted against the recorded BHT. The best fit regression through each cluster of points and the gradient of this is used as a measure of the degree of agreement between predicted and observed values. The chi-squared value, a measure of statistical validity for each regression line, for all three heat flow scenarios is above the 0.7 that is regarded as being the threshold for statistical reliability. Analysing the misfit between predicted BHT and measured BHT, it is found that on average the low heat flow scenario is 0.64 °C cooler; the mid heat flow scenario has average misfit 15.4 °C higher and the high heat flow scenario has an average misfit of 31.3 °C higher. With increasing heat flow, the corresponding gradient of the regression line through that cluster of points also increases, as does the Y-intercept. The optimum desired gradient that would be expected for best agreement between predicted and observed temperatures would verge on 1, and from this initial forward modelling it is seen that the highest heat flow scenario is closest to this. However, it is also the case that the optimum regression should be seen to pass through the origin of the cross plot and increasing the heat flow moves each regression further away from this.

Figure 5.9: Cross plot of BHT against predicted temperatures (T_{pred}) for each of the three forward modelling starting conditions for heat flow (low; mid and high case corresponding to 60; 70 and 80 mW m^{-2} respectively). With increasing input heat flow a corresponding increase is seen in the gradient of the regression line through that set of points.

Deriving heat flow across the model area (Fig. 5.10), gives mean heat flow of 60.05 mW m^{-2} and a median of 62.82 mW m^{-2} . The effective range of heat flow is between 40 & 70 mW m^{-2} .

Observing the heat flow variation across the area (Fig 5.10a) certain wells are seen to have much lower heat flow than their immediate vicinity. Consequently, during interpolation, these wells are seen in a bulls-eye zone of depressed heat flow. The most prominent of these is observed to the south west, with two wells (30/5-1 & 30/8-2) having depressed heat flow. Referring to Fig. 5.1 these two wells do not coincide with any field. The other prominent heat flow depression is found to the northeast of the model area at the intersection between Troll-A and Troll-B. The north-westernmost and easternmost wells (29/3-1 & 32/4-1, respectively) (Fig. 5.10a) influence the immediate vicinity by elevating the heat flow interpolated here.

Figure 5.10: Inverse modelling of heat flow at each well location from BHT and TVD. (a) This data is used to kriging heat flow across the model area. Kriged heat flow shows lateral variability at much higher resolution than published global grids. (b) Histogram of heat flow modelled for each well with summary statistics.

The result of running a final iteration of forward modelling for temperature with the continually laterally varying heat flow derived in Fig. 5.10 is shown in Fig. 5.11. We find when cross plotting predicted temperatures from this final model against BHT that the general distribution of points has a far tighter spread than in the previous modelling instances. The average misfit between predicted BHT and measured BHT is 0.58 °C. Furthermore, the best fit regression through this set of points has a gradient nearly equal to 1, and passes nearest to the origin, as is expected for the model best reflecting the actual subsurface temperature. Interestingly, the average of the inverse modelled heat flow as stated earlier is nearly equal to the low case heat flow input scenario used in the early stage forward modelling. Looking at the distribution of well points (Fig. 5.11) however it is clear that there is a great disparity in the two approaches. The visual impact of the two approaches is shown in Fig. 5.12d&e.

Figure 5.11: Cross plot of BHT against predicted temperatures (Tpred) with model results using inverse modelling of heat flow across the area displayed (green squares). It becomes

apparent from the chi-squared for this regression that not only is there a good statistical fit, the results have a gradient verging on 1:1 as would be expected for results best reflecting the actual subsurface temperature conditions. Furthermore, the spread of points is much narrower for this modelling outcome.

The result from the final iteration of the temperature model overlain with key structures is shown in Fig. 5.12a. Running an RMS amplitude extraction for thermal conductivity on a reference horizon (Fig. 5.12c), in this case the BCU, it is observed that the highest thermal conductivities are observed in the heart of the Viking Graben, where the BCU is deepest (Fig. 5.12b). On the flanks of the graben and eastward towards the Horda Platform, thermal conductivities are seen to decrease considerably, consistent with the increasingly shallowing BCU surface at that point. Reverting to the temperature model outputs, we see the difference between the initial forward modelling approach (Fig. 5.12d) and the final inverse modelled heat flow influenced iteration (Fig. 5.12e). Comparing the temperatures, within the deep graben for example, it is immediately apparent there is greater variation and detail discernible in from this latter approach. Indeed, what is seen is that some anomalous temperature zones are seen in this final iteration at the northern tip of the Troll field that seem to directly correlate with the anomalous heat flow zone from the interpolation (see Fig. 5.10a).

Figure 5.12: (a) Final temperature model produced using inverse modelling of heat flow overlain on transect A-A' (with well paths and BCU displayed). (b) BCU in depth with 500 m interval contours shown. (c) RMS amplitude extraction of derived thermal conductivity at BCU. (d) Low case prediction of temperature along BCU. (e) Final temperature prediction using inverse modelled heat flow along BCU. Comparing with (d) some differences are apparent. Bulls eye like temperature anomalies in the north east are likely the translation of the interpolated heat flow (see Fig. 5.10a).

The results of simulating the thermal profile for the Northern Lights test well 31/5-7 (Eos) are shown in Fig. 5.13, with temperature at bottom hole of 97 °C falling well within the projected 100 °C range published on the project website (see: <https://northernlightscs.com/en/about> accessed at 25/07/2020). Data released by Equinor and the Norwegian government in October 2020 with preliminary results indicated temperature at the bottom of 103 °C. The final well

report with its BHT record has not yet been made public but preliminary results from the 31/5-7 prediction show a good agreement between model prediction and reality.

Figure 5.13: Modelled subsurface temperature at well 31/5-7 (Eos) (see Fig. 5.1) as part of the Northern Lights CCS project. “Golden zone” for sandstone reservoirs is also displayed for context. BHT displayed is from October 2020 Eos data release of preliminary results, indicating that prediction is in close agreement with what was discovered downhole.

5.7 Discussion

There are multiple corollaries of modelling for subsurface temperature in this manner. The seismic led method of deriving subsurface thermal conductivity structure should enable the verification of zones of thermal blanketing (Cercione & Pollack, 1991; Wangen, 1995). Due to the direct relationship between velocity and thermal conductivity as used here, any zones of anomalously high or low velocity will be reflected in thermal conductivity anomalies.

However, lithologies that deviate from our general trend (which includes sandstone, shale, limestone and crystalline rocks), such as halite will need to be considered explicitly to represent the temperature above, within and below such anomalous bodies.

The benefit of the highly detailed FWI velocity model available in this area is that the velocity data has been calibrated against wells in the NVG, thus ensuring the velocity model is a good representation of true subsurface properties and conditions. The conversion to thermal conductivity and temperature provides another means of visualising the subsurface. It is of critical importance to both petroleum exploration and carbon sequestration in the area. In other locations such estimates would be highly beneficial to geothermal or gas storage operations. It must be noted that any artefacts in the velocity data will be translated to the derived thermal conductivity, instantaneous geothermal gradient and predicted temperature volumes as a consequence of the direct transitions in the workflow.

5.7.1 Heat flow modelling – impact and implications

The validation of the inverse modelling of heat flow as an input as opposed to the use of a discrete integer value heat flow input is borne out by the results. The interpolation of heat flow over the 12000 km² model area (Fig. 5.10a) highlights the variation in heat flow magnitude laterally at a much higher resolution than most existing studies. As shown earlier (Fig. 5.4), global and regional compilations usually produce heat flow grids that are at the scale of 1-degree grid squares or larger. The lateral resolution is thus many orders of magnitude poorer than when based on BHT and conductivity data. Interpolating heat flow at such fine scale might enable the examination of any trends, if any, in heat flow versus features that may be hydrocarbon fields, or structural trends (for example major fault networks). While there is a paucity of data points in the International Heat Flow Database coinciding with large parts of the Northern and Central North Sea, the many decades of hydrocarbon exploration in the area

led to numerous wells, many of which have detailed records of BHT. When combined with the seismic velocity driven model to ascertain thermal conductivity structure, it should allow for the possibility to fill in the large gaps in the global point heat flow database, which in turn should allow for more detailed basin scale heat flow studies.

The thermal anomaly visible in the interpolated heat flow map (Fig. 5.10a) can be seen to coincide with the Troll Field (Fig. 5.1). Records of this thermal anomaly attribute it to transient effects of uplift caused by late Quaternary deglaciation (Cornford, 1998). The method used to interpolate heat flow might have an impact. IDW gives the best results when the sampling is sufficiently dense with respect to the local variation being simulated (Watson & Philip, 1985). Where sampling is sparse or uneven, the interpolated result will insufficiently represent the desired surface (Philip & Watson, 1982). From the density of wells around existing fields in the area, we can be sure that the IDW interpolation will reliably capture the laterally varying heat flow at this local scale. Nonetheless at the edges of the model area there will be some degree of uncertainty associated with the interpolated heat flow, a consequence of the sampling sparseness in these regions. Kriging would be a more statistically rigorous method of interpolating heat flow, but it requires a prior investigation of the spatial behaviour of heat flow in the sample points. This is incumbent on a pre-existing understanding of the factors influencing the modelled parameter. In a blind test the latter would not necessarily be possible, and thus IDW should be satisfactory for a first order interpretation.

While heat flow has been derived from inverse modelling, in sedimentary basins there is a thermal contribution linked to the radiogenic heat production of sediments and crustal material, and the contribution of heat from the earth's deep interior (that is mantle) (Allen & Allen, 2013; Hasterok et al., 2011; Hasterok, 2010; Hokstad et al., 2017). The modelling here estimated present-day subsurface temperatures using a steady state approximation (Eq. 1). As such, a conscious decision was made to introduce as few variables as possible. Radiogenic

heat production would be one such variable. Its impact here has been noted but not explicitly modelled. Mantle heat production is usually estimated from the Moho, whose depth in the area averages roughly 30 km (Grad & Tiira, 2009). Estimates of the Curie isotherm at its shallowest in the study area place it at similar average depths of ~30 km (Fichler et al., 2011; Kubala et al., 2003). Under the graben, Moho depth does become shallow, up to 22 km in places (Licciardi et al., 2020). Referring to Fig. 5.10a, modelled heat flow is higher towards the graben centre, which suggests some correlation. With the thermal model base set at 5.5 km, and the degree of shallowing of the Moho not exceeding ~22 km at its shallowest point, the impact of mantle heat input from a modelling perspective is considered negligible in this instance. The general Moho trend in the northern North Sea has a gradual shallowing in the north-west, near the Shetland Islands (Licciardi et al., 2020). If conducting thermal modelling over the whole NVG survey area, and with the basal limits for the model set sufficiently deep such that there might be a basal mantle heat flow effect due to proximity to the Moho for the deepest section of the model.

5.7.2 Relevance

The applications of this newly validated workflow range from immediate usage by the hydrocarbon industry to supporting new subsurface uses aligned with the energy transition. Hydrocarbon explorationists may use the knowledge of the isotherms to help develop their petroleum systems models or it can help production teams better ascertain the distribution of temperature in the reservoir in order to inform reservoir engineering projects to maximise recovery. Knowledge of subsurface thermal structure is important for the nuclear waste disposal industry due to the sensitivity of the waste to thermal perturbations (Brigaud et al., 1992). From a renewable energy solutions perspective, mapping subsurface isotherms may

enable geothermal energy prospecting and the understanding of subsurface temperature will be important for CCS operations in both frontier and mature basins.

Simulating temperatures for the current CCS test well 31/5-7 emphasises the real-world applicability of this model, both in terms of its speed of producing an estimate and its relevance in the energy transition for the future. It is important to understand the temperature conditions in CO₂ storage reservoirs as the properties of the gas vary with temperature and pressure. Of these only the pressure is routinely estimated based on seismic data (Eiken et al., 2011). At higher temperatures the density of CO₂ decreases, theoretically allowing for a greater volume of it to be stored in a reservoir. Studies of CO₂ injection into the Utsira field have shown that reservoir temperature is a source of uncertainty as it can also impact the diffusivity of the gas within the reservoir (Chadwick et al., 2006). By using the subsurface thermal model proposed here, this key uncertainty may be constrained by project planners, both giving more constraint on the volume of CO₂ able to be sequestered within a reservoir, but also the ability to ascertain lateral temperature variability would enable more nuanced storage across different parts of a reservoir. Finally understanding the temperature conditions and where the potential of CO₂ diffusivity is highest could help mitigate the possibility of CO₂ leakage.

It is not just industrial applications for which this methodology may be utilised. Academic end use cases are also envisioned. The study of the microorganisms endemic to the deep subsurface is nascent and opens up the possibility of the crust playing host to potentially great biodiversity and biomass (Basso et al., 2005). Limited studies into the microbial organisms found in oil reservoirs have yielded surprising results. One such study in the Troll field, examining the microbial diversity of produced water, indicated that these microbes were not introduced as contaminants into the reservoir as a by-product of drilling; instead RNA analyses and gene matching has indicated that these are a distinct genera of temperature sensitive

microbes that do not match existing known mesophiles or thermophiles (Dahle et al., 2008). Due to the temperature dependence of these novel microbes, and the difficulty with sampling, an understanding of subsurface conditions might help in providing some inclination of the exact genera that can be encountered in a reservoir based on the predicted temperatures from the model. Thus, it is envisioned that the proposed model can assist the microbiological community as well. Bacterial remediation has been studied as a means of clean up for chemical or hydrocarbon contaminated reservoirs or aquifers (Hazen, 1997). Understanding of the temperature field in the subsurface can help determine how conducive the conditions are to the proliferation of such organisms. From a resource perspective microorganisms have been found to impact natural gas, carbon sequestration, hydrocarbons or even interfere with the underground storage of nuclear waste (Christofi & Philip, 1997).

5.8 Conclusion

The work outlines a novel methodology that utilises state of the art velocity model data from a mature basin such as the North Viking Graben to determine present day subsurface temperatures non-invasively. Forward modelling simulations underpinned by the velocity data and utilising an empirical thermal conductivity transform have been calibrated against recorded temperature data from oil field wells in this sector of the North Sea. Existing work using well data allows the computing of the vertical component of heat flow, in the same orientation as the well. Through inverse modelling here it has been demonstrated that multi axis computing of heat flow is possible with the lateral heat flow variability shown at much higher resolution than existing heat flow datasets. Using this derived heat flow to iteratively update the forward model produced a temperature model, the calibration results for which indicate the validity of this approach. To prove the real world efficacy of this work it has been applied to a recently drilled carbon capture and sequestration well, estimating the temperature in the target reservoir to be within a 5 °C margin at ~3 km subsurface depth,

highlighting the usability and robustness of this methodology in hydrocarbon exploration and future energy transition projects.

5.9 References

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5.10 Appendix

Table 5.1: Some examples of reported geothermal gradient and heat flow for the NVG and surrounding basins from the literature.

Source	Geothermal gradient (°C/km)	Heat flow (mW m ⁻²)
(Harper, 1971)	29.7	49.8 – 62.0
(Evans, 1977)		63
(Brigaud et al., 1992)	31.8 – 36.3	50 – 65
(Leadholm et al., 1985)	30 – 35	58.6 – 67
(Justwan et al., 2006)		52.3
(Cornford, 1998)		60 – 82
(Lucazeau & Le Douaran, 1985)		65
(Goff, 1983)	32	57 – 65
(Rüpke et al., 2008)	30 – 40	
(Ritter et al., 2004)		65

6. Impact of velocity input in seismic thermometry

6.1 Abstract

Subsurface temperature fields are traditionally determined from direct measurements. However, indirect means of determining subsurface temperature fields can be a useful supplement or even substitute in the absence of borehole and heat flow records. One such avenue uses seismic velocity data as input combined with either surface or subsurface temperature or heat flow calibration. In a previous study, this seismic thermal modelling, or seismic thermometry, process was investigated in the mature North Sea basin, using a detailed full waveform inversion (FWI) velocity model covering the North Viking Graben (NVG). In a follow up to this work, the impact of varying the velocity input on the temperature predictions has been examined, with the final FWI velocity contrasted against a fast track residual move out (RMO) velocity model. Ample borehole constraint in the NVG allows for the cross examination of results and allows an assessment of whether it is possible to derive and apply a correction factor to the predicted temperature, depending on the input velocity type. Considering this, results from the seismic thermometry process carried out in the frontier Lüderitz Basin, offshore Namibia are revisited, with the temperature prediction adjusted by ± 3 °C in accordance with the derived temperature correction factor.

6.2 Non-invasive approach to subsurface temperature modelling: state of play and previous modelling

Determining subsurface temperature offshore can be done through direct means which has often involved drilling of boreholes into which tools for temperature measurement can be lowered (Beardmore & Cull, 2001). Understanding temperature in the subsurface can help

numerous end use cases such as the determination of source rock effectiveness in hydrocarbon exploration (Faraji et al., 2019); geothermal energy prospecting (Bonté et al., 2012); carbon capture and sequestration efforts (Chadwick et al., 2006; Cozier, 2019) as industrial applications. For the scientific community subsurface isotherms could help in the understanding of organisms adapted to unique conditions (Dahle et al., 2008; Purkamo et al., 2020) or model for the potential impacts of gas hydrate dissociation and the contribution to climate change (Kretschmer et al., 2015; Ruppel, 2011; Ruppel & Kessler, 2017) or instigating slope instability related mass movement of sediment (Gabitto & Tsouris, 2010; Lemon, 2012; Solheim et al., 2005). Clearly there exists great interest in temperature fields in the subsurface. As stated earlier, most existing tools involve direct measurement, but this can be costly and difficult especially in deep water settings. Over time methods have been investigated to determine temperature through either non-invasive means (seismic reflection data) or from the transformation of existing physical properties logs (such as density; porosity; sonic logs). The former approach (dubbed “seismic thermometry”) is favoured here and has been explored by these authors in previous studies offshore Namibia (Sarkar & Huuse, 2021b); offshore USA (Sarkar & Huuse, 2021c); and in the North Sea (Sarkar & Huuse, 2021c). Using seismic reflection and velocity data, temperature in the subsurface was resolved using a one-dimensional approximation of Fourier’s Law, with thermal conductivity derived from an empirical relationship with velocity. Deriving thermal conductivity in this manner has been explored through laboratory based studies in the past (Duffaut et al., 2018; Gu et al., 2017; Jorand et al., 2015; Mielke et al., 2017) and has guided the approach here. The North Viking Graben (NVG) in the North Sea has ample borehole data to constrain the results of the modelling. Calibration indicates that the results of modelling for temperature in this manner compare favourably to bottom hole temperatures (BHT) (Sarkar & Huuse, 2021c). However in all the previous instances that the authors conducted this modelling workflow, the velocity

data utilised has varied, with seismic processing velocities available in Namibia (Sarkar & Huuse, 2021b); vertical seismic profiler (VSP) data in the Blake Ridge (Sarkar & Huuse, 2021c); and both fast track residual move out (RMO) & full waveform inversion (FWI) velocity data available for the work conducted in the NVG (Sarkar & Huuse, 2021c). In this latter case the FWI velocities were utilised for the proof of concept modelling due to their greater level of detail and agreement with borehole data utilised to build the velocity model. The question that raised itself was to what extent does the choice of velocity data affect the calculated temperatures. Any velocity input influenced trends observed might then be used to determine if the temperature prediction made in the frontier Lüderitz Basin will then warrant adjusting.

Figure 6.1: (a) North Viking Graben (NVG) study area with thermal model subset area and calibration wells shown. (b) Lüderitz Basin study area shown. Bathymetry from GEBCO (*"The GEBCO_2019 Grid - a continuous terrain model of the global oceans and land,"* 2019)

6.2.1 Geological setting

Two offshore basins, the North Sea Basin and the Lüderitz Basin will be referred to in this work.

6.2.1.1 North Viking Graben (NVG)

The primary study area is in the NVG, part of the northern North Sea basin, a mature and prolific petroleum province. The graben was formed from the initiation of rifting and thermal subsidence in the Permo-Triassic, likely through reactivation of existing structures (Glennie & Underhill, 2009). The graben system trends northward (Keym et al., 2006) with five NNE trending half grabens forming an en echelon pattern (Copestake et al., 2003). Sub basins formed in these half grabens with large rotated fault blocks bounded by NNE-SSW and NE-SW trending faults. These sub basins and rotated fault blocks became buried by Cretaceous and Cenozoic sediment, which formed multiple isolated kitchen areas each of differing thermal maturity due to their differing individual subsidence and uplift histories (Keym et al., 2006). Pre-rift deltaic sandstones of the Middle Jurassic Brent Group make up the excellent reservoir rocks found in these fault blocks (Johannesen et al., 2002).

6.2.1.2 Lüderitz Basin

The Lüderitz Basin, offshore Namibia, is part of a volcanic passive margin (Gladczenko et al., 1998; Light et al., 1993; Wanke & Toirac-proenza, 2018). It is a frontier deep-water basin. Multiple rifting events from the Carboniferous onwards occurred, with the South Atlantic opening in the Mesozoic (Bagguley & Prosser, 1999; Schmidt, 2004). Diachronous reopening suggests a pre-existing line of weakness (anisotropy) facilitated new rifting. This rifting was also asymmetric in character, with the conjugate margin in Brazil varying considerably in its sedimentary and subsidence history (Mello et al., 2013). Due south of the volcanic Walvis Ridge, the basins offshore Namibia were not affected by the restricted marine conditions created by it during the Albian-Aptian, and thus no salt is encountered (Davison & Underhill, 2012). Given the absence of salt in this basin, the corresponding thermal impact of salt tectonics are also negated.

6.2.2 Data

Figure 6.2: West-east transect (Fig. 6.1a) from the NVG with schematic overlay of major structural features and stratigraphic horizons showing (a) Average velocity (V_p) from FWI volume of FWI model; (b) Average velocity from fast track RMO volume of RMO model.

6.2.2.1 Seismic data

Seismic data available for the NVG included a 2017 vintage high resolution 3D seismic volume (both reflection and velocity) covering 35410 km^2 (courtesy of CGG). The velocity data includes a fast track velocity volume in time (consisting of root mean squared (RMS) stacking velocities) and an FWI volume that is migrated for both time and depth (PSTM and PSDM). Acquisition parameters are summarised in Table 6.1. The fast track velocities formed the starting point for the iterations of tomographic update and model building used to arrive at the final FWI

velocity model. This latter model underpinned the modelling work discussed in Sarkar & Huuse (2021c).

Table 6.1: Acquisition parameters for CGG's "3DKjempe" survey covering the Northern North Sea (CGG, 2019), and Polarcus' 3D survey covering the Lüderitz Basin, offshore Namibia (NAM).

Acquisition parameters	NVG survey	NAM survey
Area size (km ²)	35410	4150
TWT down to (s)	9	9.2
Sample interval (ms)	2	4
Bin spacing (m)	6.25×18.75	12.5×25
Line separation (m)	75	50
Shot point interval (m)	18.75	25
Shooting pattern	Flip flop	Flip flop
Streamers	12	10
Streamer length (m)	7950	8100
Tow depth (m)	6 & 9	6
Streamer separation (m)	75	100
Dominant frequency (Hz)	~40 - 50	40

Both 2D and 3D seismic reflection data was available for the Lüderitz Basin, with four 2D lines totalling 752 km and a 3D volume of area 4150 km². The 2D data is PSTM & PSDM while the 3D data is pre stack time migrated (PreSTM), with reprocessing in 2012 used to produce a smooth velocity volume.

6.2.2.2 Borehole data

Borehole data from the Norwegian Petroleum Directorate (NPD) was used to calibrate the results for the NVG, with a subset of 139 oil and gas exploration wells used (Fig. 6.1a). In the Lüderitz Basin there is limited well control with a solitary Ocean Drilling Program (ODP) borehole (1084) in the distal deep water and a lone oil & gas exploration well on the proximal shelf (Norsk Hydro 2513/8-1) (Fig. 6.2b). These do not provide sufficient opportunity for

temperature calibration, hence the significance of assessing whether the temperature estimates are sensitive to the velocity data used.

6.3 Contrasting velocity input on thermometry output

6.3.1 Previous work – final velocity product models

The thermal modelling workflow utilised in this work is shown in Fig. 6.3 and has been previously explored by the authors (Sarkar & Huuse, 2021-a; -b; -c). It is reliant on the conversion of seismic velocity data to thermal conductivity using an empirical transform derived from experimental data. There is precedent in the academic record for the utilisation of other physical properties to determine thermal conductivity (Gu et al., 2017; Schön, 2015; Zamora et al., 1993). The thermal conductivity transform is bespoke and has been compiled from published experimental data with the goal to cover the broadest suite of porosities encounterable in the subsurface (and by association, the broadest range of common lithologies). This empirical transform is as follows:

Equation 1: $k_v = (6 \times 10^{-5})V_p^{1.3279}$

Where k_v is thermal conductivity from velocity ($\text{W m}^{-1} \text{K}^{-1}$) and V_p is P wave velocity (m s^{-1})

The thermal structure of the subsurface is determined using a one-dimensional approximation of Fourier's Law, shown below:

Equation 2: $Q = k \times \frac{dT}{dZ}$

Where Q is heat flow (mW m^{-2}); k is thermal conductivity ($\text{W m}^{-1} \text{K}^{-1}$) and dT/dZ is geothermal gradient ($^{\circ}\text{C km}^{-1}$).

Figure 6.3: Simplified procedure for seismic data derived thermal modelling, alongside summary workflow for steps required to condition fast track seismic processing velocity data for use in seismic thermometry process in the North Sea example.

To enable comparison of the thermal modelling products from different velocity input for the NVG, heat flow is assigned a constant value of 60 mW m^{-2} . This heat flow was found to be best representative for the model area based on nearby measurements from the international heat flow database (Gosnold & Panda, 2002) and published estimates in global studies (Davies,

2013; Lucazeau, 2019). In a previous study (Sarkar & Huuse, 2021a), using thermal conductivity from the best representative velocities (FWI) and BHT from each well, heat flow was individually modelled, thus giving an inverse modelled heat flow across the area. This is considered a more precise representation of laterally varying heat flow and as such it informs the best case subsurface thermal model. This model serves as a point of reference for the comparative models. It shall be referred to as Inverse Q model.

6.3.2 Conditioning fast track velocities

As stated earlier the fast track residual move out (RMO) velocities are in fact stacking velocities. The model workflow uses average velocities as a starting point and thus the RMS stacking velocities must undergo Dix conversion to interval velocities first. Following Dix conversion, the resulting instantaneous velocities in time domain, will have some spurious values. The RMS velocities were picked to purely optimise the stacking process so conversion can be unstable. The fast track velocities were picked for the purposes of migration and thus do not have high velocities nor the level of detail in terms of geobodies that is evident from the FWI velocity product. The coarse converted velocity volume must undergo vertical smoothing at this stage. Smoothing was an iterative process, with the early smoothing conducted with the same filter settings. The structural smoothing operation used on Petrel is a spatial smoothing operator underpinned by a weighted Gaussian filter, in which the filter size represents the standard deviation of the applied Gaussian filter. The bigger the filter width, the greater the number of traces and samples over which operation is conducted. Later iterations of smoothing used larger filter settings. In total four successive iterations of smoothing were applied. Time limitations enforced the number of smoothing iterations and ever-increasing filter windows utilised. Ideally many more iterations of smoothing with a small window each time would have been run to arrive at the final product best resembling the FWI

volume used in the previous study. Once smoothing has been completed, a velocity model is created, from which an average velocity volume is derived. This velocity product may now be used in conjunction with Eq. 1 to derive a thermal conductivity volume. The remaining workflow follows the same procedures outlined in Fig. 6.3.

Figure 6.4: (a) Noisy interval velocity output for the NVG from the Dix conversion of fast track RMO velocity model. (b) Fast track interval velocities after undergoing multiple smoothing iterations to remove noise.

6.4 Calibration and contrast

Table 6.2: Reference key for the models being discussed

Model	Input velocity model	Heat flow input
FWI model	Final FWI velocities	Constant (60 mW m ⁻²)
RMO model	Fast track RMO velocities	Constant (60 mW m ⁻²)
Inverse Q model	Final FWI velocities	Laterally varying inversely modelled heat flow

6.4.1 Calibrating against recorded data

Bottom hole temperatures (BHT) from 139 wells within the study area have been used for calibrating the temperatures obtained from the velocities. There are two temperature models being compared: one using the FWI velocities as a starting point and the other using the fast track RMO velocities (refer to Table 6.2 for model nomenclature). For each of these models, synthetic temperature logs for the calibration wells are created, thereby allowing synthetic/predicted BHT to be plot against the recorded BHT value. These results (Fig. 6.5a) show that RMO model (black crosses) has a greater spread of results compared to FWI model (blue circles). Using a linear regression through each corresponding cluster, it becomes clear that the fast track RMO velocity based prediction has a steeper gradient than the model using the FWI velocities. Ideally for a positive correlation with real BHT, the gradient of any regression should be 1 and the fit should pass through the origin and this is what is seen for Inverse Q model (green squares). This is the best-case prediction and is displayed to give context for the models being compared. The gradient of the best fit regression for RMO model is closest to the best case, though both FWI model and RMO model show similar goodness of fit on the basis of their chi-squared values.

Figure 6.5: (a) Cross plot of predicted temperatures from each model for the NVG (FWI model; RMO model; Inverse Q model), against measured BHT for each calibration well. (b) Fast track RMO velocity based model results plotted directly against the final FWI velocity model results.

6.4.2 Contrasting temperature output

To put the results in context of the stratigraphy of the North Sea, they have been displayed against the base Cretaceous unconformity (BCU) (Fig. 6.6). RMO model (Fig. 6.6b) has by far the greatest spread of temperatures across the BCU, followed by Inverse Q model (Fig. 6.6c) and finally FWI model (Fig. 6.6b), which has the smallest range. Focusing on the graben to the west, it becomes apparent that RMO model predicts the warmest temperatures, up to 40 °C warmer than seen for FWI model. To better visualise the disparity in temperatures predicted by the FWI- and RMO- models, the temperature difference between the two models is shown (Fig. 6.6d). What this shows is that on average predicted temperature from RMO model is 18 °C warmer than the results from FWI model. Visualising this on a histogram there is a bimodal distribution. Moving towards the flanks of the graben there is little to no difference between the predictions from either model, it is only in the graben centre itself that there are great disparities, which in turn leads to the smaller secondary peak in the histogram.

Figure 6.6: RMS amplitude temperature extractions along the base Cretaceous unconformity (BCU) in the NVG area for (a) FWI model (FWI based, constant heat flow); (b) RMO model (RMO based, constant heat flow); (c) Inverse Q model (FWI with inverse modelled heat flow). (d) FWI model minus RMO model temperatures shown along BCU with accompanying histogram of values (right).

6.4.3 Comparing input velocities

Previously the temperature output from each model was contrasted against each other. This shows there are clear differences in the output that must be linked to the velocity input (as the other variables such as input heat flow and thermal conductivity transformation are the same across both FWI- and RMO- models). As thermal conductivities are based upon the average rather than interval velocities, the average velocity profile for each borehole is computed for both models. These results are shown in Fig. 6.7a. From the shape of the best fit regression, at lower velocities there is good agreement between both RMO and FWI velocities. But with increasing velocity, RMO velocities increase much less with depth than the FWI velocities.

Figure 6.7: (a) Average velocities contrasted for FWI- and RMO- models. Polynomial fit is forced through origin and excludes isolated highest velocity points in interests of curve fitting. (b) Interval velocities for a subset of 3 wells compared against each other for the fast track and final velocity models. (c) Interval velocity from FWI velocity model compared against sonic log data. (d) Interval velocity from RMO velocity model compared against sonic log data.

6.5 Implications for velocity input on seismic thermometry process

There would appear to be a link between the type of velocity input and the temperature prediction output by the seismic thermometry process. This is clear from the results of the FWI- and RMO- models comparing the effect of the fast track velocities against a much more detailed final FWI velocity product. To compare the two velocity models directly, certain sense checks are necessary. As borehole data is available for the NVG, sonic log data should be present. In future, an early check would thus be to contrast sonic log results against the interval velocities for both models. What was compared earlier was the average velocity across the borehole length for each well from both input velocity models. In the context of rock physics properties, it is instead interval velocity that will be more directly linked to these properties. Thus, any checkshot based data or sonic logs for example will correlate with interval velocities in principle. Ideally such a quality control check would be done for all 139 wells used for calibration but for the interests of time, it has been done for three wells, selected from one of three major hydrocarbon fields in the area (Fig. 6.7c, d). As would be expected for the FWI velocities (Fig. 6.7c), they show good correlation with sonic log velocity. This is because the final FWI velocity model is calibrated against the borehole velocity data. But for fast track velocities there is poorer correlation with sonic across all three wells, especially at greater depths.

Comparing the interval velocities across both velocity models directly against each other (Fig. 6.7b), there is strong correlation, as expected because the FWI volume is created iteratively from processing velocities and well velocity data.

6.5.1 Potential correction factor

As is clear from Fig. 6.5a, temperatures are overpredicted using the fast track RMO velocities as they convert to lower thermal conductivities when applying the transform. When directly

correlating the outputted temperatures against each other (Fig. 6.5b), it was found that the RMO based result (RMO model) overpredicts temperature when using the FWI based result (FWI model) as calibration. Mapping the temperature predictions along a stratigraphic marker (BCU) (Fig. 6.6) also allows more trends to be discernible. To further examine this, the attributes mapped along the BCU (Fig. 6.6c – best case temperature prediction; Fig. 6.6d – ΔT , where $\Delta T = \text{Measured } T - \text{Predicted } T$) are converted to points, and then plotted against each other (Fig. 6.8). Some immediate trends become apparent, with the temperature output differential from the two kinds of velocity input (ΔT) plotted against actual temperature (considered the Inverse Q model output as it calibrates closest to the BHT) (Fig. 6.8a), and against BCU depth (Fig. 6.8b). The depth trend that was first noticed in Fig. 6.6d is more clearly evident here, with the highest temperature differential seen in the graben also corresponding to the greatest depths. There appears a threshold depth of roughly 2400 m after which there is a proportional relationship between depth and the extent to which model outputs have varied based on velocity input. Similarly, when comparing to temperature, there appears to be a threshold temperature of 100 °C, after which a similar proportional pattern of increase between temperature and ΔT is observed. What might be the cause of such clear trends related to temperature and depth are not yet clear. Given the similarity of the observed trends and the link to the different velocity input, it is likely then that there is some relation between depth and the velocity models, specifically the manner in which they were constructed. While this does not yield a conclusive direct relationship for a velocity input based correction factor, it is an intriguing result. This could be an area of future investigation.

Figure 6.8: (a) ΔT (where $\Delta T = \text{Measured } T - \text{Predicted } T$; see Fig. 6.6d) plotted against the best-case temperature prediction (see Fig. 6.6c). This shows that the greatest divergence between the FWI and RMO based temperature output corresponds with temperatures above a $\sim 100^\circ\text{C}$ threshold point. (b) ΔT (see Fig. 6.6d) plotted against BCU depth (see Fig. 5.12b). As shown previously, the greatest divergence in model output corresponds with depths greater than $\sim 2400\text{ m}$, following a near linear trend.

6.5.2 Revisiting the Lüderitz Basin

Seismic thermometry modelling had previously been conducted in the Lüderitz Basin (Sarkar & Huuse, 2021b). The input velocities in this instance are seismic processing velocities. As seen so far, the velocity input will affect the temperature prediction. Processing velocities will be closer to a fast track velocity model than an FWI model like used in FWI model & Inverse Q model. If so, it stands to reason that the temperature at the bottom hole is overpredicted when compared to the actual BHT. In the Lüderitz Basin the single borehole calibration

available is a proximal shelfal borehole (2513/8-1) with BHT which have had a simple correction applied (<https://www.zetaware.com/utilities/bht/lastresort.html> first accessed August 2018). Though not as reliable as the BHT data from the NVG study, it provides some indication of subsurface temperature conditions here and gives context for results from the seismic thermometry process.

As seen in 6.5.1, no conclusive evidence was found for a simple correction factor based on velocities itself. However, it is clear that there is a relation between the velocity input type on the thermal model output. Using the direct thermal output contrast between FWI model & RMO model (see Fig. 6.5b) as a guide, a simple correction was derived as follows:

$$\text{Equation 3: } T_{RMO} = 1.2109 \times T_{FWI}$$

Where T_{RMO} is thermometric output based on RMO velocity input (°C) and T_{FWI} is thermometric output based on FWI velocity input (°C).

This has been applied as a correction factor for temperature prediction used for the Namibia study, resulting in the predicted temperature curve shifting (Fig. 6.9)

Figure 6.9: Previously modelled results from application of seismic thermometry to the Lüderitz Basin with 95% upper and lower confidence bounds. A correction factor (derived from the NVG study) has been applied to the initial velocity input and the resulting temperature curve (cyan) is shifted to the left.

The application of the temperature correction factor has the overall effect of shifting the subsurface temperature prediction curve towards the cooler end. In the process the resulting predictions are still within the lower confidence bound of the previous Namibia study, whilst also corresponding to the corrected BHT. It diverges from the corrected BHT points by ± 3 °C.

6.6 Conclusions

Seismic thermometry presents a means of estimating temperatures in the subsurface using seismic velocity modelling data. This has been tested in the NVG. The type of velocity data available for input impacts the predicted temperature, with a fast track RMO velocity model leading to overprediction of temperature compared to recorded BHT. In comparison a detailed final FWI velocity model leads to temperature predictions that are in better agreement with the BHT. Cross correlating the temperature prediction results of the two different input velocity models, a preliminary correction factor has been identified which may be used to condition input velocities for use in the seismic thermometry process. This correction factor, when applied to a pre-existing study in Namibia shows that it will shift the temperature curve. Further studies using different velocity inputs in the seismic thermometry process with physical data constraint from borehole data will allow for a theoretical correction curve that can be applied globally for the input in such a modelling procedure.

6.7 References

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7. Synthesis

In chapter 1, the aim of this project to investigate and develop a novel approach to determine subsurface temperatures was outlined. Chapter 2 summarised the current state of play with regard to subsurface temperature in terms of our understanding of the factors influencing temperature conditions in the crust; the primary mechanisms by which heat is generated and the approaches in which these thermal conditions are measured. The various techniques and tools for direct measurement have been highlighted. The fundamental concepts of heat transfer and the relationship between key thermal properties such as heat flow; thermal conductivity and geothermal gradient are also discussed to provide context for the development of the novel approach in this work. To this end, a brief summary of gas hydrates is given, as the early investigations as part of this project developed upon pre-existing workflows using the identification of BSRs as an isotherm. The other key pillar to this work has been the deriving of thermal conductivity from velocity data and the experimental studies that have underpinned this particular part have also been discussed in chapter 2. In the course of technical chapters 3 – 6, three case studies were conducted using offshore datasets in Namibia, USA and the North Sea to develop the methodology; test it; calibrate it and showcase how it may be applied to both frontier and mature areas. These studies were conducted over the course of 4 years through collaborative work involving industry partners at the Basins Research Group facilities at the University of Manchester. Industry partners such as Serica, Spectrum (now TGS); CGG and Schlumberger were instrumental in providing both the data and software with which this project was completed.

This final chapter will seek to summarise the findings of the technical chapters, framing them in context of their contribution to the understanding of temperature in the subsurface and the avenues for future work that may result from this project.

7.1 Pathways to remote sensing subsurface thermal conditions

Over the course of the technical chapters 3 – 6, the methodology for reflection seismic thermometry has been both developed iteratively and refined. The workflow is displayed in Figs. 3.5, 4.4, 5.5 & 6.3. For each of those case studies there was a requirement for adaptation to the methodology due to the available dataset. In chapter 3 (see section 3.3), input data included both a seismic reflection volume and a processing velocity volume though there was extremely limited well control, thus obviating any possibility for calibration. In chapter 4 (see section 4.4), input data included reflection seismic data and borehole control was present in the form of ODP boreholes. But velocity input here was in the form of borehole velocities (VSP data). For the final case study covered in chapters 5 & 6 (see sections 5.5 & 6.2.2, respectively), both seismic reflection and seismic velocity data were available with abundant well control. Here however the critical difference was the absence of observable BSRs on seismic. Nonetheless in Fig. 7.1 below, an attempt has been made to summarise the principal pathways that form part of the reflection seismic thermometry process.

Figure 7.1: Summary workflow for the reflection seismic thermometry procedure, as applied across this project. The various key constituent steps of the process are listed and present various avenues in terms of starting conditions from which to derive a subsurface thermal model (which is the primary deliverable for this work). Intermediate output has been considered as the heat flow proxy from BSR or the inverse modelled heat flow can both be considered as input for heat flow focussed studies for example.

The reference to pathways in Fig. 7.1 has been made as it is felt that the composite workflow shown above can be considered in terms of subset processes nested within the process, each of which can produce a deliverable that may be utilised separate from the primary deliverable, that is the subsurface temperature model.

7.1.1 Shallow thermal regime

The first such subset pathway to consider can be dubbed the shallow thermal regime process. This work is fundamentally underpinned by the presence of a BSR on seismic and the pressure-temperature linked stability conditions of the hydrate that cause it. As such this is an avenue that has been tested and utilised widely in the literature (Burwicz & Rüpke, 2019; Calvès et al., 2010; Grevenmeyer & Villinger, 2001; Serié et al., 2017; Shankar et al., 2014; Shankar & Riedel, 2013; Vargas-Cordero et al., 2010). The key steps here are the identification of the BSR at the base of the GHSZ on reflection seismic data. If the depth of the BSR is known, it is possible to use the pressure-temperature relationship of its stability field (example Fig. 3.9b; Fig. 4.7f) to define an isotherm along it (Dickens & Quinby-Hunt, 1994; Lu & Sultan, 2008; Sloan, 1990; Tishchenko et al., 2005). In chapter 3, there is a lack of constraint on the exact composition of the hydrate present in the Lüderitz Basin due to the lack of information from the nearby ODP 1084 borehole (Wefer et al., 1998). Therefore, the relationship of Dickens & Quinby-Hunt (1994) was adapted and utilised to determine temperature at the BSR isotherm:

$$T_{BSR} = ((3.79 \times 10^{-3} - 2.83 \times 10^{-4}(\log(\rho \times g \times Z_{BSR})))^{-1}) - 273$$

Where T_{BSR} is the temperature at GHSZ (°C); ρ is density (kg m⁻³) (of seawater); g is acceleration due to gravity (m s⁻²) and Z_{BSR} is the depth (m) of the BSR.

Due to many detailed studies targeting the hydrates at Blake Ridge (Bryan, 1974; Burwicz & Rüpke, 2019; Egeberg & Dickens, 1999; Guerin et al., 1999; Holbrook, 2001; Hornbach et al., 2003; Kvenvolden & Barnard, 1982; Max & Dillon, 1999; C. Paull et al., 1995; Taylor et al.,

2000), there is confidence in the hydrate composition in this area. As such the experimental hydrate stability relationship of Lu & Sultan (2008) was preferred to determine the temperature at the BSR in chapter 4. The adapted relationship is as follows:

$$T_{BSR} = \frac{(\ln P - \ln F_s - E_s S)}{C_s S + D_s} - 273$$

Where T_{BSR} is temperature at the BSR (°C); P is pressure (MPa); S is salinity; F_s , C_s , D_s & E_s are empirical constants: $F_s = 1.010769956 * 10^{-9}$; $C_s = 0.1711726397$; $D_s = 0.1046133676$; $E_s = -34.14836102$; respectively.

If the temperature at seabed is known, available. from NOAA databases (such as the WOA) (Locarnini et al., 2013), then it becomes possible to compute a shallow geothermal gradient as the thickness of the hydrate stability zone is known.

$$\frac{dT}{dZ} GHSZ = \frac{T_{BSR} - T_{SEABED}}{Z_{BSR} - Z_{SEABED}}$$

Where dT/dZ is geothermal gradient (°C km⁻¹); T_{BSR} is temperature at BSR (°C); T_{SEABED} is seabed temperature (°C); Z_{BSR} is depth of BSR (km); Z_{SEABED} is seafloor depth (km).

At the onset (see section 2.2) it was shown that the fundamental relationship linking the thermal properties of thermal conductivity, thermal gradient and heat flow is given by Fourier's Law of heat conduction.

$$Q = k \times \frac{dT}{dZ}$$

Where Q is heat flow (mWm⁻²); k is thermal conductivity (W m⁻¹ K⁻¹) and dT/dZ is geothermal gradient (°C km⁻¹).

In this work, it is a 1D approximation of this law that is utilised at the various stages to derive the desired thermal property. As part of the shallow thermal regime component of the workflow, there is an intermediate deliverable (Fig. 7.1) that is a BSR derived heat flow proxy. If thermal conductivity is known, either through direct measurement data from boreholes, or

through derivation from an alternative physical property (this being velocity data as discussed in section 7.1.2), then it becomes possible to use the shallow geothermal gradient computed for the GHSZ & Fourier's Law to derive heat flow. This kind of heat flow data differs from traditional point based heat flow datasets (such as that available from the International Heat Flow Commission (Gosnold & Panda, 2002) or from ODP/IODP (Pribnow et al., 2000)) in its link to seismic data. That is, it is derived from the identification of a BSR on seismic reflection data, and since the BSR is identified across either a solitary 2D transect or 3D seismic grid, it then follows that the heat flow should also be valid laterally across the same directions as the source seismic (Calvès et al., 2010; Martin et al., 2004; Priyanto, 2018; Shankar & Riedel, 2013). Thus, unlike traditional point-based heat flow data, there is less of a need for extrapolation in 2D or 3D space for heat flow when using this BSR derived heat flow proxy. This makes it more attractive for use, especially in offshore settings that may be constrained by the availability of borehole data vis-à-vis seismic data.

7.1.2 Primary thermometry pathway

The principal input data for this work is velocity data, be it seismic velocities or based on borehole measurements. To understand how velocity data is transformed in a manner that is input into the thermometric model it is crucial to understand the empirical transform between velocity and thermal conductivity. This is covered in chapter 2 (section 2.3.4). Essentially over time, many indirect means of determining temperature (section 2.3.3) have been pursued, some of which have included looking at the Curie isotherm for example (Blakely, 1988; Rajaram et al., 2009). Earlier it was mentioned how Fourier's Law is key to simplifying the necessary constituents for the seismic thermometry process. From the shallow thermal regime pathway, a BSR can be used to determine a shallow geothermal gradient and heat flow may be available from another source, thus leaving thermal conductivity as the remaining

variable. Traditionally thermal conductivity is ascertained from direct measurements (see section 2.3.4.1) either in the borehole or on samples in a laboratory (Beardsmore & Cull, 2001; Gunn et al., 2005; Popov et al., 1999; Williams & Anderson, 1990). However, the premise of this work is for an offshore setting lacking borehole control, thus it is unlikely that thermal conductivity data will be available. The difficulty of gathering and having access to thermal conductivity data is a quandary that has led authors in the past to explore means to determine it from other more easily acquired physical data (see section 2.3.4.2), such as velocity logs for example (Esteban et al., 2015; Gegenhuber & Schoen, 2012; Griffiths et al., 1992; Pimienta et al., 2018; Zamora et al., 1993). There is precedent then in the use of empirical relationships to derive thermal conductivity from another property, in this case acoustic velocities (Eberhart-Phillips et al., 1989). Mining the published record for experimental studies with both thermal conductivity and velocity data, a point cloud was iteratively populated over the course of the project. The development of this point cloud and the best fit regression used to define the empirical transform used can be seen in each of the technical chapters (see Figs. 3.6; 4.5; 5.6). Common parameters for the input data including ensuring samples were all wet at time of measurement and used similar (transient) measuring techniques such as an optical scanner for example. It must be noted that the empirical relationship is designed such that it should give a reliable approximation of the bulk thermal conductivity and has been compiled as such and tested thus far in passive margin settings. In active tectonic settings, the point cloud for the transform might require adjusting.

In the final NVG study the empirical transform is:

$$k_V = (6 \times 10^{-5})V_p^{1.3279}$$

Where k_V is thermal conductivity from velocity ($\text{W m}^{-1} \text{K}^{-1}$) and V_p is P wave velocity (m s^{-1}).

The transform can be applied to either interval or average velocities, and for computational reasons average velocity and conductivities were used for the continuous temperature estimation. This is because temperature is cumulative and always increases downwards unless encountering specific plumbing or advection circumstances.

7.1.2.1 Velocity input types

Velocity input is needed as the starting condition for the seismic thermometry process. Over the course of the project, different kinds of velocities have been tested with the workflow, which has served to highlight the versatility of the proposed methodology. Seismic velocities have been used in chapters 3, 5 & 6 covering the Namibia and North Sea case studies. In the absence of seismic velocities, borehole (VSP) velocities (Holbrook et al., 1996) were substituted (chapter 4). While acoustic velocities, whatever their format, when input into the seismic thermometry workflow output a temperature product, it raised the question of what impact different velocity format would have on the final product. This is the aim of chapter 6, which uses the detailed velocities available in a well constrained area of the northern North Sea to examine what effect would be there (see section 7.2).

7.1.3 Bulk geothermal gradient and heat flow conditioning

Referring to Fourier's Law again, all that is required for the seismic/borehole velocity derived bulk thermal conductivity volume to transform to geothermal gradient is heat flow. For the purposes of this project, the fundamental diversion from a traditional basin modelling approach has been to consider the impact of heat flow from a top down approach (from the surface-water interface) than a bottom up approach (from a basal heat flow boundary such as the Moho). At the onset of this project, one motivation was to pursue the application of this to help petroleum exploration. In such a scenario, key deliverables would be to determine the temperature conditions for a target horizon (that can either be a reservoir or a source

interval). This target horizon is simply put, likely to be much closer to the sediment water interface than the basal isotherm such as Moho (Mareschal & Jaupart, 2013). It is felt then that heat flow for the uppermost sections of the crust (i.e. closest to the seabed in this project) would be satisfactorily representative for the thermal model output. Also, it must be noted that the component of radiogenic heat production (see section 2.1), has not been modelled for its contribution to the thermal model.

Under the heat flow assumptions outlined above, it becomes clear how the shallow BSR-derived heat flow proxy can serve to condition the bulk thermal gradient. This has been applied in chapters 3 & 4. This approach would present a wholly remote sensing aspect to the reflection seismic thermometry process, with no borehole data input required at any stage, thus representing the purest non-invasively acquired results. In offshore continental margin settings with conducive conditions for the development of gas hydrates and observable BSRs on seismic reflection data, it presents the ideal scenario for ascertaining temperature.

However, for the North Sea study (chapter 5), the crucial difference is the lack of a BSR in the NVG. This necessitates a change in procedure for the heat flow conditioning of the bulk thermal gradient volume. There are two distinct possibilities that have been explored here. Under the premise of a blind test, where the borehole data is considered to be available only after the modelling has been conducted, it becomes necessary to have a pre-set heat flow input. This can be either a best guess or based on alternate heat flow databases and published literature. The resulting final subsurface model when calibrated against available borehole temperatures, presents the opportunity where an iterative loop can be set up. Taking inspiration from the FWI model building process of the NVG seismic velocity model data in chapter 5 (where seismic velocity models are iteratively updated till the difference between observed and modelled seismic waveforms is minimised (Warner et al., 2013)), the heat flow input can be iteratively updated. Here the analogy for the observed waveform is the observed

temperature (i.e. BHT) and the modelled waveform is the subsurface temperature model (Tpred). Giving an example scenario, in the frontier stage of a basin, the thermometry model will be built using the pre-set heat flow input (provided no BSR is available to derive a heat flow proxy). Subsequently as exploratory boreholes are drilled and their results become available, calibration of the model can be conducted, with each new borehole (and its accompanying temperature data) available used to both further constrain the subsurface thermal model but also to adjust the heat flow conditioning at the bulk thermal gradient stage. This should then, over time allow the subsurface thermal model to verge on what is actually occurring over a basin.

But the North Sea is prolifically drilled, and thus there is ample borehole constraint here. Bizarrely, as shown in Fig. 5.4, there is a conspicuous absence of open source heat flow data coverage over the NVG. Given the abundant hydrocarbon well data over this same interval, an inverse modelling scenario presented itself. Operating under the assumption that the recorded borehole temperatures are valid, and that the seismic velocity volume and the empirical thermal conductivity transform are both valid, it should be possible to compute heat flow for each borehole. This is what has been done as well in chapter 5. Coupled with the seismic thermal conductivity process, it presents the possibility for the seismic thermometry process to deliver laterally varying shallow heat flow data output in addition to temperature. this inverse modelled heat flow then is another possibility for conditioning the bulk thermal gradient volume.

Once the bulk thermal gradient has been arrived at, the procedure to create the final subsurface thermal model is simple.

$$T = T_{SEABED} + \left(\frac{dT}{dZ} \times Z_{SUBSURFACE} \right)$$

where T is predicted temperature ($^{\circ}\text{C}$); T_{SEABED} is the temperature at seabed ($^{\circ}\text{C}$); dT/dZ is the instantaneous geothermal gradient ($^{\circ}\text{C km}^{-1}$) (Equation 2); and $Z_{SUBSURFACE}$ is the subsurface depth (km).

At this stage the final subsurface temperature model is available for either calibration against available borehole data or for the end user to derive temperature attribute maps for intervals of interest for example.

7.2 Case study results summarised

Three primary case studies have been conducted over the course of this project (see section 2.5.1). The results of each of these are displayed in Fig. 7.2. The results shall be discussed in context of the rationale for the project as presented in chapter 1.2.

As the first available dataset, the methodology was initially developed and tested in the Lüderitz Basin (chapter 3). Here a distinct BSR (Swart, 2009) was identified on both 2D and 3D seismic reflection data. Using the earliest iteration of the empirical thermal conductivity transform, seismic processing velocities for this study area were used to produce a bulk thermal conductivity volume. This helped in defining a BSR derived shallow heat flow proxy result (63.8 mW m^{-2}) that is considered particularly useful for this passive, volcanic margin setting due to the lack of borehole data control in the immediate vicinity. This lack of borehole control presented difficulties in terms of calibrating the results. As such a set of pseudo wells were modelled to examine the temperature trends from the thermometric model (Fig. 7.2a). From a petroleum systems perspective, key queries in this area remain the effectiveness of the Aptian source interval. At an average temperature of 133.5°C , it is in the gas generative window. This is consistent with the same interval producing gas in the Kudu field to the south. Due to the lack of borehole constraint, the workflow remained uncalibrated at the onset of chapter 4. Here it was sought to test in a similarly deep-water passive margin setting that had

ample constraint on the nature of the gas hydrates present and accompanying borehole control. This was chosen to be the Blake Ridge, offshore USA. With the nature of the gas hydrate and BSR in this location extensively studied and understood, the shallow thermal regime pathway was tested and verified against ODP Leg 164 data. However seismic velocities were lacking, and thus the results are presented in terms of 1D models at the borehole locations (Fig. 7.2b). Laterally varying heat flow derived from the BSR was also produced (Fig. 4.7e). A principal benefit of this modelling has been the extending the knowledge of subsurface thermal regime in this area up to 330 m deeper than the existing ODP thermal profiles.

The final case study in the North Sea had access to the highest resolution, high fidelity velocity data in the form of a state of the art FWI velocity model. With velocity data the principal input in the seismic thermometry process (Fig. 7.1) it is no surprise that the highest confidence velocity input from the NVG corresponds to the highest confidence results from this project in chapters 5 & 6. The key aim here was to conduct a blind test of the workflow utilising this FWI velocity model to calibrate against borehole temperatures (BHT) (chapter 5). Using defined heat flow input, it was found the thermal output calibration well with the BHTs. However inverse modelling heat flow with the aid of the BHT and the empirical transform for thermal conductivity, presented a map of heat flow for the study area (Fig. 5.10a). Compared to existing heat flow grids for this area (Davies, 2013; Lucazeau, 2019), heat flow derived in this manner is found to have a lateral resolution far exceeded the former. Using this heat flow to condition the bulk thermal gradient yields results that match closest to the BHT.

A corollary of the varying vintages of velocity data available for the NVG (a fast track RMO velocity volume and the final FWI velocity volume) and the abundant well control presented the opportunity to examine how differing seismic velocity input types would impact the seismic thermometry results. This forms the premise for chapter 6. As can be expected, the

FWI velocities, calibrated against the observed subsurface conditions in the form of 101 boreholes during the model building stage, are found to yield temperatures closest to the BHT when calibrating. Basing the predicted temperatures on RMS/stacking type velocities had the general effect of over estimating temperatures by up to 30 °C. In light of this finding, the Namibian results from chapter 3 were revisited. Here the velocity input consisted of seismic processing velocities. Thus, it is likely that the model result would overpredict the temperatures in the subsurface here, particularly at the depth of Prospect B, a 570 km² volcanoclastic carbonate build up believed to be of Barremian age (Rochelle-Bates et al., 2017). The analysis suggests that in this case the size of the overestimate is only a few degrees.

Figure 7.2: (a) The global workflow (see Fig. 7.1) as adapted for chapter 3 (blanked out portions indicate those inputs and processes not valid for this particular study) and a west-east transect with the final temperature model overlay (right). Three pseudo wells (shown on the inset map) are also displayed with their results shown in Fig. 3.12b. This was the first application of the reflection seismic thermometry process, in a frontier basin. Plan view top reservoir (Prospect B) map inset with 200 m depth contours and temperature displayed.

Figure 7.2 (cont.): (b) The global workflow (see Fig. 7.1) as adapted for chapter 4 is shown (left) alongside the 2D seismic line (95-18-01) from the Blake Ridge, with the ODP boreholes 994, 995 & 997 from Leg 164. As the seismic thermometric models were built using the borehole (VSP) velocities here, the temperature output is displayed along the well paths, with the BSR demarcated for reference (solid red – observed on seismic; dotted red – inferred).

Figure 7.2 (cont.): (c) The global workflow (see Fig. 7.1) as adapted for chapter 5 is shown (left) alongside transect A-A' from the NVG (inset map below with calibration wells and 3D survey extent shown). Reflection seismic data is overlain with the thermal overlay, highlighting the change in temperatures and how they correspond to major structures (BCU is shown for reference with solid black marker on reflection seismic). Plan view map is for top BCU depth surface with predicted temperature displayed.

7.3 Implications

The principal outcome of this work is the validity of the reflection seismic thermometry process. It presents an avenue to greatly enhance our existing understanding of the thermal structure of the subsurface, especially offshore. Using the overall workflow (Fig. 7.1) as a guide, it becomes possible to demarcate those areas in which there have been gains to the current knowledge, with implications in terms of disparate end use cases.

7.3.1 Industrial applications

It is evident that pursuing the purely remote sensing approach will be very beneficial to frontier hydrocarbon exploration as demonstrated in chapter 3. For sure areas, especially deep-water settings, where challenging operating conditions and external pressures might reduce the possibility of drilling wildcat wells, such an approach can aid the explorationist in terms of reducing the uncertainty in petroleum systems elements such as the source and reservoir (Allen & Allen, 2013). As seismic reflection data quality and its reach has expanded (both in terms of geographical spread and the depths to which it extends, often in excess of borehole data), this methodology would provide seismic operating companies additional value to their libraries. This is essentially what has been shown in chapters 5 & 6, where a modern seismic dataset has been used in a mature basin. Thus, in addition to frontier exploration, this process can aid near field exploration in areas such as the North Sea. This should enable more efficient recovery (Awan et al., 2006) and utilisation of the existing hydrocarbon resources in terms of further delimiting the subsurface isotherm structure.

The proposed methodology can just as easily be adapted to aid in the energy transition. As shown in chapter 5, it was relatively simple to model the temperature field for the Eos well, part of the Northern Lights CCS program (Cozier, 2019). Understanding the temperature field

in storage reservoirs can help project planners better ascertain the storage volumes they can expect, and where there might be potential for leakage (Ringrose, 2020; Vilarrasa & Rutqvist, 2017). With geophysical monitoring of such storage reservoirs already a precedent (Chadwick et al., 2006; Eiken et al., 2011), it should simply be a case of plug-and-play for the reflection seismic thermometry process to be added to these workflows. Similarly, it can be envisioned that this process is applied to aid geothermal energy prospecting.

7.3.2 Scientific applications

Chapter 4 exclusively used open source data, primarily from the ODP. It was demonstrated how for offshore continental margin ODP locations that intersect a BSR, and have borehole velocity data in the form of VSP or sonic logs, it is possible to derive a thermogram where there is none, or extend the thermal profile that already exists. This could be a valuable tool. With a small percentage (~43%) of the cumulative ODP database having reliable temperature data (Pribnow et al., 2000), but a greater proportion of these boreholes likely to have reliable velocity logs, it presents the opportunity to greatly enhance the ODP repository for thermal data. Given researchers outside the geoscience community take advantage of such datasets, this presents the opportunity for this seismic thermometric process to contribute to multidisciplinary research. An example would be the study of temperature adapted biota by the microbiological community (Basso et al., 2005; Dahle et al., 2008).

BSRs have already been demonstrated to help derive heat flow by past authors (Grevemeyer & Villinger, 2001; Horai & Von Herzen, 1985; Hornbach et al., 2020; Phrampus et al., 2017; Uyeda & Horai, 1982). Thus, the shallow heat flow output is not particularly novel. What can be considered novel is the inverse modelling procedure for heat flow demonstrated in chapter 5. Coupled with hydrocarbon well data and seismic derived thermal conductivity, it becomes possible to quantify heat flow in basins that might not be of interest from a heat flow study

perspective, and thus currently lacking such data in global compilations/data repositories. This can have the effect of expanding the existing knowledge of heat flow in offshore basins with heat flow modelled in this manner having the additional benefit of having a lateral resolution corresponding to the seismic input data, which is often at far greater detail compared to existing compilations.

7.4 Future work

Whilst the aims and objectives set out in Chapter 1 have largely been met, there is still more work to do to validate and further constrain the methodology, boundary conditions and transform, especially when transporting and testing this on different settings. Consequently, there remains certain areas for future work to be conducted.

One such area is to fully explore the entire NVG dataset from chapters 5 & 6. The thermal model covered a subset of the whole survey area with a subset of the wells within used to calibrate. The natural extension would be to extend the model area to the entirety of the survey, making use of as many boreholes that fall within for calibration. This should help to further refine the temperature models produced and the thermometry process too. In turn this should provide scope for a detailed study to refine the component steps of the workflow for the uncertainty linked to it as well as the cumulative uncertainty of the thermometry process. This uncertainty analysis was briefly conducted in chapters 3 & 4 but would benefit from the greater well control and better input data in the NVG case study.

Further to this, in chapter 4, the analysis of the impact of the differing velocity input utilised three wells to contrast due to time constraints. With more time available it would be in the interests of this line of investigation to extend the comparative analysis across as great a proportion of the 139 calibration wells used in chapter 5. It is expected that this should help give more conclusive evidence of the overall contrast between the RMO and FWI velocity

models as input for thermometry, whether this reinforces the trend ascertained in chapter 6 or not.

The empirical thermal conductivity transform is a key component of the overall reflection seismic thermometry process. As stated in this project, it is something that has been iteratively developed over the course of the project. It should continue to be developed, tested and refined in the future with the addition of more data and the exclusion of others, to get the best representative estimate. One possibility that has been thought of is utilising the borehole data, for example in the NVG. Should temperature data be available at various depth points along the well path, it becomes possible to estimate thermal conductivity for the intervals between these temperature-depth pairs, creating a layer cake thermal conductivity model. It should be examined how the cross plot of velocity and thermal conductivity used to derive the empirical transform would be affected by inputting these aforementioned thermal conductivity interval data.

Given the increasing importance of CCS as part of the energy transition, it is hoped that some collaborative work can be conducted. Colleagues in the Basins Group are working with the same NVG dataset (from chapters 5 & 6), focusing on the Utsira formation in this case. It should be possible to apply the methodology to target the reservoir itself and produce detailed temperature fields within it as part of a joint paper.

This leads on to the potential for further case studies in offshore settings with this methodology. In Appendix 1, a co-authored publication is included for the Baffin Bay, offshore Greenland, where part of the methodology has been utilised to derive heat flow in a frontier basin.

It is evident from the applications listed above that there is ample scope for the proposed methodology. Some authors (Wu et al., 2020) have demonstrated the ability of using the

tertiary seismic arrivals from earthquakes to derive basin scale deep ocean temperature. With the quantification of thermal regime a requirement for numerous hot button issues, the nascent field of reflection seismic thermometry (as proposed in this work) has the possibility to become an important avenue of research moving forward.

7.5 References

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Appendix 1 – Standard thermal conductivity values in the literature

Figure 8.1: Thermal conductivity for assorted common rock types after (Cermak & Rybach, 1982; Mielke et al., 2017; Rybach & Bunterbarth, 1982)

Mineral	Thermal conductivity (W/m/K)	Source reference (s)
Quartz	7.69	Horai (1971)
Calcite	3.6	Horai (1971); Cermak and Rybach (1982)
Dolomite	5.6	Popov et al. (1999)
Pyrite	19.2	Horai (1971)
Haematite	11	Horai (1971)
Halite	5.50	Smith (1976)
Smectite	1.88	Brigaud and Vasseur (1989)
Kaolinite	2.6	Brigaud and Vasseur (1989)
Chlorite	3.3	Horai (1971); Brigaud and Vasseur (1989)
Illite	1.9	Brigaud and Vasseur (1989)
Mixed-layer clays I/S	1.9	Brigaud et al. (1992)
Biotite	2.09	Horai (1971)
Muscovite	2.30	Horai (1971)
Alkali feldspar microcline	2.4	Horai (1971); Popov et al. (1999)
Water	0.6	Clauser and Huenges (1995)
Air	0.025	Clauser and Huenges (1995)

Figure 8.2: Compilation of thermal conductivity from (Esteban et al., 2015)

Figure 8.3: Thermal conductivity (here λ) ternary diagram for key rock forming minerals with their compositional relation with rock type. (a) Metamorphic and plutonic rocks. (b) Volcanic and sedimentary rocks. Due to the importance of porosity for thermal conductivity in volcanic or sedimentary rocks, the third 'mineral' phase is referred to as air or water. From (Özkahraman et al., 2004)

Mineral	V_p (m s ⁻¹)	λ (W m ⁻¹ K ⁻¹)	A_{solid} (W s ² m ⁻³ K ⁻¹)
Quartz	6050	7.5	0.21×10^{-6}
Olivine	8550	3.1	0.04×10^{-6}
Pyroxene	7700	4.5	0.08×10^{-6}
Hornblende	6810	2.8	0.06×10^{-6}
Feldspar (mean)	4680	2.0	0.09×10^{-6}
Muscovite	5810	2.3	0.07×10^{-6}
Biotite	5350	2.0	0.07×10^{-6}
Calcite	6640	3.6	0.08×10^{-6}
Dolomite	7340	5.5	0.10×10^{-6}
Anhydrite	5640	4.8	0.15×10^{-6}

Figure 8.4: Velocity and thermal conductivity (here λ) compilation from (Schön, 2015)

Appendix 2 – Raw data for empirical thermal conductivity transform

Figure 8.5: Velocity-thermal conductivity cross plot with all the raw data used in this project. From (Boulanouar et al., 2013; Duffaut et al., 2018; Esteban et al., 2015; Grevemeyer & Villinger, 2001; Gu et al., 2017; Hartmann et al., 2005; Jorand et al., 2015; Leadholm et al., 1985; Mielke et al., 2017)

Vp [m s ⁻¹]	Thermal conductivity [W m ⁻¹ K ⁻¹]	SOURCE
5217	3.008	Boulanouar et al., 2013
6080	2.805	Boulanouar et al., 2013
6095	3.085	Boulanouar et al., 2013
6160	3.115	Boulanouar et al., 2013
3300	1.89	Boulanouar et al., 2013
3250	1.781	Boulanouar et al., 2013
3180	2.083	Boulanouar et al., 2013
3200	1.973	Boulanouar et al., 2013
4370	2.504	Boulanouar et al., 2013
4440	2.622	Boulanouar et al., 2013
4350	2.525	Boulanouar et al., 2013
5070	2.54	Boulanouar et al., 2013
4164	2.643	Boulanouar et al., 2013
1614.658	1.22406	Villinger & Grevemeyer, 2001
1628.822	1.217143	Villinger & Grevemeyer, 2001
1631.52	1.220752	Villinger & Grevemeyer, 2001
1648.157	1.269474	Villinger & Grevemeyer, 2001
1654.901	1.231579	Villinger & Grevemeyer, 2001
1652.203	1.218045	Villinger & Grevemeyer, 2001
1635.567	1.194286	Villinger & Grevemeyer, 2001
1651.304	1.196692	Villinger & Grevemeyer, 2001
1652.878	1.190677	Villinger & Grevemeyer, 2001
1656.7	1.191278	Villinger & Grevemeyer, 2001
1654.002	1.211128	Villinger & Grevemeyer, 2001
1659.847	1.193384	Villinger & Grevemeyer, 2001
1660.747	1.199098	Villinger & Grevemeyer, 2001
1663.444	1.188572	Villinger & Grevemeyer, 2001

1666.592	1.206015	Villinger & Grevemeyer, 2001
1663.669	1.210226	Villinger & Grevemeyer, 2001
1664.568	1.221353	Villinger & Grevemeyer, 2001
1668.39	1.222256	Villinger & Grevemeyer, 2001
1670.414	1.199098	Villinger & Grevemeyer, 2001
1672.212	1.202707	Villinger & Grevemeyer, 2001
1671.987	1.206917	Villinger & Grevemeyer, 2001
1675.135	1.199098	Villinger & Grevemeyer, 2001
1674.46	1.178947	Villinger & Grevemeyer, 2001
1685.926	1.183459	Villinger & Grevemeyer, 2001
1679.856	1.199699	Villinger & Grevemeyer, 2001
1680.081	1.206316	Villinger & Grevemeyer, 2001
1684.577	1.205113	Villinger & Grevemeyer, 2001
1687.275	1.202406	Villinger & Grevemeyer, 2001
1688.399	1.216241	Villinger & Grevemeyer, 2001
1692.221	1.196692	Villinger & Grevemeyer, 2001
1692.446	1.190075	Villinger & Grevemeyer, 2001
1696.718	1.187068	Villinger & Grevemeyer, 2001
1698.067	1.17594	Villinger & Grevemeyer, 2001
1700.09	1.173534	Villinger & Grevemeyer, 2001
1701.664	1.159699	Villinger & Grevemeyer, 2001
1696.268	1.205414	Villinger & Grevemeyer, 2001
1697.842	1.213233	Villinger & Grevemeyer, 2001
1700.09	1.217744	Villinger & Grevemeyer, 2001
1700.989	1.210226	Villinger & Grevemeyer, 2001
1676.034	1.24812	Villinger & Grevemeyer, 2001
1691.322	1.259549	Villinger & Grevemeyer, 2001
1699.191	1.268872	Villinger & Grevemeyer, 2001
1707.734	1.276692	Villinger & Grevemeyer, 2001

1710.207	1.268872	Villinger & Grevemeyer, 2001
1706.61	1.256241	Villinger & Grevemeyer, 2001
1704.137	1.225263	Villinger & Grevemeyer, 2001
1706.385	1.223459	Villinger & Grevemeyer, 2001
1712.005	1.232782	Villinger & Grevemeyer, 2001
1720.324	1.241504	Villinger & Grevemeyer, 2001
1711.781	1.225564	Villinger & Grevemeyer, 2001
1714.703	1.223759	Villinger & Grevemeyer, 2001
1719.649	1.221053	Villinger & Grevemeyer, 2001
1713.579	1.216842	Villinger & Grevemeyer, 2001
1709.308	1.214135	Villinger & Grevemeyer, 2001
1712.905	1.212632	Villinger & Grevemeyer, 2001
1707.959	1.194587	Villinger & Grevemeyer, 2001
1710.881	1.182857	Villinger & Grevemeyer, 2001
1714.029	1.177444	Villinger & Grevemeyer, 2001
1716.277	1.178647	Villinger & Grevemeyer, 2001
1737.86	1.138045	Villinger & Grevemeyer, 2001
1751.574	1.138647	Villinger & Grevemeyer, 2001
1758.543	1.129624	Villinger & Grevemeyer, 2001
1773.606	1.138647	Villinger & Grevemeyer, 2001
1759.442	1.150075	Villinger & Grevemeyer, 2001
1730.441	1.181955	Villinger & Grevemeyer, 2001
1724.82	1.18406	Villinger & Grevemeyer, 2001
1720.099	1.208722	Villinger & Grevemeyer, 2001
1725.495	1.210526	Villinger & Grevemeyer, 2001
1728.867	1.203609	Villinger & Grevemeyer, 2001
1731.115	1.200301	Villinger & Grevemeyer, 2001
1741.682	1.18797	Villinger & Grevemeyer, 2001
1743.48	1.193083	Villinger & Grevemeyer, 2001

1752.248	1.187669	Villinger & Grevemeyer, 2001
1758.543	1.189774	Villinger & Grevemeyer, 2001
1767.311	1.186767	Villinger & Grevemeyer, 2001
1752.023	1.198196	Villinger & Grevemeyer, 2001
1741.457	1.205113	Villinger & Grevemeyer, 2001
1734.038	1.209624	Villinger & Grevemeyer, 2001
1732.914	1.220451	Villinger & Grevemeyer, 2001
1729.541	1.250226	Villinger & Grevemeyer, 2001
1731.565	1.251729	Villinger & Grevemeyer, 2001
1734.263	1.254737	Villinger & Grevemeyer, 2001
1733.588	1.258045	Villinger & Grevemeyer, 2001
1733.588	1.263158	Villinger & Grevemeyer, 2001
1730.665	1.266767	Villinger & Grevemeyer, 2001
1737.185	1.242406	Villinger & Grevemeyer, 2001
1741.007	1.221353	Villinger & Grevemeyer, 2001
1743.031	1.226466	Villinger & Grevemeyer, 2001
1748.651	1.224662	Villinger & Grevemeyer, 2001
1752.023	1.225865	Villinger & Grevemeyer, 2001
1748.426	1.243308	Villinger & Grevemeyer, 2001
1750.45	1.250827	Villinger & Grevemeyer, 2001
1751.124	1.267669	Villinger & Grevemeyer, 2001
1760.567	1.254135	Villinger & Grevemeyer, 2001
1761.466	1.250226	Villinger & Grevemeyer, 2001
1762.815	1.246316	Villinger & Grevemeyer, 2001
1763.04	1.257143	Villinger & Grevemeyer, 2001
1761.466	1.202707	Villinger & Grevemeyer, 2001
1764.613	1.205414	Villinger & Grevemeyer, 2001
1767.086	1.213835	Villinger & Grevemeyer, 2001
1777.203	1.194286	Villinger & Grevemeyer, 2001

1781.475	1.146165	Villinger & Grevemeyer, 2001
1790.468	1.151579	Villinger & Grevemeyer, 2001
1789.568	1.133534	Villinger & Grevemeyer, 2001
1790.917	1.130827	Villinger & Grevemeyer, 2001
1796.763	1.135639	Villinger & Grevemeyer, 2001
1797.887	1.132932	Villinger & Grevemeyer, 2001
1800.36	1.13203	Villinger & Grevemeyer, 2001
1803.282	1.137744	Villinger & Grevemeyer, 2001
1806.43	1.135338	Villinger & Grevemeyer, 2001
1816.322	1.136541	Villinger & Grevemeyer, 2001
1800.585	1.150677	Villinger & Grevemeyer, 2001
1800.585	1.154586	Villinger & Grevemeyer, 2001
1794.065	1.168722	Villinger & Grevemeyer, 2001
1785.522	1.176241	Villinger & Grevemeyer, 2001
1792.716	1.178346	Villinger & Grevemeyer, 2001
1785.297	1.185865	Villinger & Grevemeyer, 2001
1779.676	1.196993	Villinger & Grevemeyer, 2001
1781.025	1.2	Villinger & Grevemeyer, 2001
1778.552	1.202406	Villinger & Grevemeyer, 2001
1778.552	1.209023	Villinger & Grevemeyer, 2001
1781.925	1.21203	Villinger & Grevemeyer, 2001
1787.095	1.211128	Villinger & Grevemeyer, 2001
1777.878	1.217744	Villinger & Grevemeyer, 2001
1780.126	1.222256	Villinger & Grevemeyer, 2001
1772.032	1.23609	Villinger & Grevemeyer, 2001
1771.808	1.248722	Villinger & Grevemeyer, 2001
1772.707	1.25985	Villinger & Grevemeyer, 2001
1781.475	1.266767	Villinger & Grevemeyer, 2001
1780.576	1.272782	Villinger & Grevemeyer, 2001

1773.606	1.290226	Villinger & Grevemeyer, 2001
1767.311	1.302556	Villinger & Grevemeyer, 2001
1796.538	1.259248	Villinger & Grevemeyer, 2001
1798.786	1.271579	Villinger & Grevemeyer, 2001
1816.997	1.274286	Villinger & Grevemeyer, 2001
1819.02	1.277594	Villinger & Grevemeyer, 2001
1825.54	1.282406	Villinger & Grevemeyer, 2001
1821.043	1.298647	Villinger & Grevemeyer, 2001
1806.655	1.32812	Villinger & Grevemeyer, 2001
1840.153	1.33203	Villinger & Grevemeyer, 2001
1849.146	1.322707	Villinger & Grevemeyer, 2001
1870.504	1.328722	Villinger & Grevemeyer, 2001
1895.908	1.326617	Villinger & Grevemeyer, 2001
1891.187	1.375639	Villinger & Grevemeyer, 2001
1902.653	1.317293	Villinger & Grevemeyer, 2001
1917.491	1.348271	Villinger & Grevemeyer, 2001
1925.36	1.329023	Villinger & Grevemeyer, 2001
1908.948	1.296842	Villinger & Grevemeyer, 2001
1914.344	1.276391	Villinger & Grevemeyer, 2001
1917.266	1.270978	Villinger & Grevemeyer, 2001
1920.638	1.272782	Villinger & Grevemeyer, 2001
1922.212	1.276391	Villinger & Grevemeyer, 2001
1931.655	1.281504	Villinger & Grevemeyer, 2001
1916.367	1.285113	Villinger & Grevemeyer, 2001
1917.941	1.295338	Villinger & Grevemeyer, 2001
1923.786	1.291729	Villinger & Grevemeyer, 2001
1926.709	1.296241	Villinger & Grevemeyer, 2001
1945.594	1.280301	Villinger & Grevemeyer, 2001
1947.167	1.284511	Villinger & Grevemeyer, 2001

1947.167	1.294135	Villinger & Grevemeyer, 2001
1943.795	1.298045	Villinger & Grevemeyer, 2001
1929.182	1.313684	Villinger & Grevemeyer, 2001
1943.795	1.313083	Villinger & Grevemeyer, 2001
1953.687	1.281504	Villinger & Grevemeyer, 2001
1955.935	1.285113	Villinger & Grevemeyer, 2001
1957.959	1.287519	Villinger & Grevemeyer, 2001
1964.029	1.28812	Villinger & Grevemeyer, 2001
1957.959	1.312481	Villinger & Grevemeyer, 2001
1975.944	1.450226	Villinger & Grevemeyer, 2001
1972.572	1.360602	Villinger & Grevemeyer, 2001
1982.239	1.305564	Villinger & Grevemeyer, 2001
1995.054	1.307068	Villinger & Grevemeyer, 2001
1986.286	1.30015	Villinger & Grevemeyer, 2001
1986.286	1.294436	Villinger & Grevemeyer, 2001
1982.239	1.294737	Villinger & Grevemeyer, 2001
1982.914	1.28812	Villinger & Grevemeyer, 2001
1986.736	1.28391	Villinger & Grevemeyer, 2001
2000.225	1.277594	Villinger & Grevemeyer, 2001
1997.302	1.271579	Villinger & Grevemeyer, 2001
1993.705	1.270075	Villinger & Grevemeyer, 2001
1990.558	1.268571	Villinger & Grevemeyer, 2001
1990.108	1.271579	Villinger & Grevemeyer, 2001
1988.085	1.273985	Villinger & Grevemeyer, 2001
1986.286	1.275188	Villinger & Grevemeyer, 2001
1984.712	1.277594	Villinger & Grevemeyer, 2001
1982.689	1.279699	Villinger & Grevemeyer, 2001
1981.34	1.283008	Villinger & Grevemeyer, 2001
1981.34	1.275188	Villinger & Grevemeyer, 2001

1983.588	1.268571	Villinger & Grevemeyer, 2001
1997.077	1.260451	Villinger & Grevemeyer, 2001
1997.077	1.254436	Villinger & Grevemeyer, 2001
1994.155	1.25594	Villinger & Grevemeyer, 2001
1991.232	1.258647	Villinger & Grevemeyer, 2001
1990.782	1.25203	Villinger & Grevemeyer, 2001
1986.061	1.253534	Villinger & Grevemeyer, 2001
1987.635	1.247218	Villinger & Grevemeyer, 2001
1988.984	1.240602	Villinger & Grevemeyer, 2001
1987.635	1.237293	Villinger & Grevemeyer, 2001
1993.031	1.244511	Villinger & Grevemeyer, 2001
1995.054	1.249323	Villinger & Grevemeyer, 2001
1993.93	1.241203	Villinger & Grevemeyer, 2001
1996.853	1.242406	Villinger & Grevemeyer, 2001
1995.054	1.228571	Villinger & Grevemeyer, 2001
1994.38	1.219549	Villinger & Grevemeyer, 2001
1992.131	1.227068	Villinger & Grevemeyer, 2001
1989.658	1.230075	Villinger & Grevemeyer, 2001
1984.263	1.233083	Villinger & Grevemeyer, 2001
1983.588	1.242707	Villinger & Grevemeyer, 2001
1984.712	1.221053	Villinger & Grevemeyer, 2001
1986.286	1.211429	Villinger & Grevemeyer, 2001
1972.122	1.227068	Villinger & Grevemeyer, 2001
1989.433	1.205414	Villinger & Grevemeyer, 2001
1993.255	1.206917	Villinger & Grevemeyer, 2001
1995.504	1.20812	Villinger & Grevemeyer, 2001
1995.953	1.202105	Villinger & Grevemeyer, 2001
1995.279	1.16782	Villinger & Grevemeyer, 2001
1995.279	1.17594	Villinger & Grevemeyer, 2001

1991.682	1.177744	Villinger & Grevemeyer, 2001
1981.115	1.179248	Villinger & Grevemeyer, 2001
1982.464	1.188271	Villinger & Grevemeyer, 2001
1979.991	1.185564	Villinger & Grevemeyer, 2001
1982.689	1.201805	Villinger & Grevemeyer, 2001
1975.944	1.201203	Villinger & Grevemeyer, 2001
1974.595	1.175639	Villinger & Grevemeyer, 2001
1966.952	1.175639	Villinger & Grevemeyer, 2001
1966.952	1.161203	Villinger & Grevemeyer, 2001
1967.176	1.15579	Villinger & Grevemeyer, 2001
1955.486	1.140752	Villinger & Grevemeyer, 2001
1943.795	1.101353	Villinger & Grevemeyer, 2001
1941.322	1.115489	Villinger & Grevemeyer, 2001
1939.074	1.139549	Villinger & Grevemeyer, 2001
1858.363	1.133233	Villinger & Grevemeyer, 2001
1843.076	1.13594	Villinger & Grevemeyer, 2001
1840.603	1.132632	Villinger & Grevemeyer, 2001
1831.385	1.133835	Villinger & Grevemeyer, 2001
1825.315	1.135038	Villinger & Grevemeyer, 2001
1827.788	1.151278	Villinger & Grevemeyer, 2001
1824.191	1.15188	Villinger & Grevemeyer, 2001
1804.631	1.173233	Villinger & Grevemeyer, 2001
1794.739	1.187669	Villinger & Grevemeyer, 2001
1789.344	1.192782	Villinger & Grevemeyer, 2001
1800.585	1.193985	Villinger & Grevemeyer, 2001
1795.863	1.197594	Villinger & Grevemeyer, 2001
1799.011	1.208722	Villinger & Grevemeyer, 2001
1794.739	1.211128	Villinger & Grevemeyer, 2001
1793.615	1.215639	Villinger & Grevemeyer, 2001

1776.529	1.246015	Villinger & Grevemeyer, 2001
1780.8	1.236692	Villinger & Grevemeyer, 2001
1782.149	1.24391	Villinger & Grevemeyer, 2001
1787.32	1.226165	Villinger & Grevemeyer, 2001
1786.646	1.234587	Villinger & Grevemeyer, 2001
1789.568	1.233684	Villinger & Grevemeyer, 2001
1792.491	1.230075	Villinger & Grevemeyer, 2001
1782.374	1.250827	Villinger & Grevemeyer, 2001
1780.351	1.253534	Villinger & Grevemeyer, 2001
1786.196	1.258647	Villinger & Grevemeyer, 2001
1789.568	1.255639	Villinger & Grevemeyer, 2001
1792.941	1.237895	Villinger & Grevemeyer, 2001
1796.088	1.233985	Villinger & Grevemeyer, 2001
1795.414	1.240602	Villinger & Grevemeyer, 2001
1798.561	1.231278	Villinger & Grevemeyer, 2001
1800.809	1.227068	Villinger & Grevemeyer, 2001
1802.833	1.226165	Villinger & Grevemeyer, 2001
1800.36	1.216842	Villinger & Grevemeyer, 2001
1801.034	1.235789	Villinger & Grevemeyer, 2001
1803.282	1.233083	Villinger & Grevemeyer, 2001
1803.282	1.235789	Villinger & Grevemeyer, 2001
1803.957	1.238496	Villinger & Grevemeyer, 2001
1804.856	1.240301	Villinger & Grevemeyer, 2001
1802.608	1.240602	Villinger & Grevemeyer, 2001
1801.259	1.241805	Villinger & Grevemeyer, 2001
1799.91	1.243609	Villinger & Grevemeyer, 2001
1799.236	1.245714	Villinger & Grevemeyer, 2001
1801.933	1.250827	Villinger & Grevemeyer, 2001
1806.88	1.254135	Villinger & Grevemeyer, 2001

1808.228	1.239399	Villinger & Grevemeyer, 2001
1807.779	1.233383	Villinger & Grevemeyer, 2001
1806.88	1.230075	Villinger & Grevemeyer, 2001
1809.353	1.234587	Villinger & Grevemeyer, 2001
1811.601	1.235789	Villinger & Grevemeyer, 2001
1812.5	1.238196	Villinger & Grevemeyer, 2001
1813.624	1.240602	Villinger & Grevemeyer, 2001
1814.973	1.242105	Villinger & Grevemeyer, 2001
1815.872	1.243308	Villinger & Grevemeyer, 2001
1817.446	1.247519	Villinger & Grevemeyer, 2001
1815.872	1.248421	Villinger & Grevemeyer, 2001
1815.423	1.256842	Villinger & Grevemeyer, 2001
1814.748	1.258647	Villinger & Grevemeyer, 2001
1808.678	1.181955	Villinger & Grevemeyer, 2001
1810.252	1.18376	Villinger & Grevemeyer, 2001
1810.477	1.184361	Villinger & Grevemeyer, 2001
1810.027	1.186166	Villinger & Grevemeyer, 2001
1809.128	1.187368	Villinger & Grevemeyer, 2001
1808.453	1.189774	Villinger & Grevemeyer, 2001
1808.453	1.193083	Villinger & Grevemeyer, 2001
1809.128	1.195489	Villinger & Grevemeyer, 2001
1812.725	1.194587	Villinger & Grevemeyer, 2001
1812.275	1.190978	Villinger & Grevemeyer, 2001
1812.725	1.202406	Villinger & Grevemeyer, 2001
1810.702	1.203609	Villinger & Grevemeyer, 2001
1810.702	1.206015	Villinger & Grevemeyer, 2001
1808.678	1.20812	Villinger & Grevemeyer, 2001
1807.329	1.209925	Villinger & Grevemeyer, 2001
1808.678	1.22015	Villinger & Grevemeyer, 2001

1810.926	1.22406	Villinger & Grevemeyer, 2001
1812.05	1.227068	Villinger & Grevemeyer, 2001
1814.748	1.229173	Villinger & Grevemeyer, 2001
1816.097	1.173233	Villinger & Grevemeyer, 2001
1819.694	1.17985	Villinger & Grevemeyer, 2001
1819.02	1.181654	Villinger & Grevemeyer, 2001
1818.345	1.183459	Villinger & Grevemeyer, 2001
1818.121	1.186466	Villinger & Grevemeyer, 2001
1818.121	1.189173	Villinger & Grevemeyer, 2001
1818.795	1.199699	Villinger & Grevemeyer, 2001
1822.392	1.201203	Villinger & Grevemeyer, 2001
1824.865	1.201805	Villinger & Grevemeyer, 2001
1827.113	1.202105	Villinger & Grevemeyer, 2001
1830.486	1.203308	Villinger & Grevemeyer, 2001
1835.432	1.204812	Villinger & Grevemeyer, 2001
1838.579	1.205113	Villinger & Grevemeyer, 2001
1830.261	1.19579	Villinger & Grevemeyer, 2001
1830.71	1.179248	Villinger & Grevemeyer, 2001
1834.308	1.154586	Villinger & Grevemeyer, 2001
1839.254	1.154286	Villinger & Grevemeyer, 2001
1844.2	1.154887	Villinger & Grevemeyer, 2001
1846.673	1.145564	Villinger & Grevemeyer, 2001
1855.665	1.140451	Villinger & Grevemeyer, 2001
1859.712	1.149474	Villinger & Grevemeyer, 2001
1863.309	1.149173	Villinger & Grevemeyer, 2001
1865.782	1.153384	Villinger & Grevemeyer, 2001
1864.658	1.156992	Villinger & Grevemeyer, 2001
1862.635	1.15579	Villinger & Grevemeyer, 2001
1858.363	1.162406	Villinger & Grevemeyer, 2001

1854.541	1.158196	Villinger & Grevemeyer, 2001
1855.216	1.154887	Villinger & Grevemeyer, 2001
1853.642	1.150376	Villinger & Grevemeyer, 2001
1850.27	1.153985	Villinger & Grevemeyer, 2001
1852.968	1.157594	Villinger & Grevemeyer, 2001
1849.595	1.172932	Villinger & Grevemeyer, 2001
1853.417	1.175038	Villinger & Grevemeyer, 2001
1840.827	1.175038	Villinger & Grevemeyer, 2001
1836.556	1.181353	Villinger & Grevemeyer, 2001
1841.277	1.179549	Villinger & Grevemeyer, 2001
1848.022	1.179248	Villinger & Grevemeyer, 2001
1838.579	1.188872	Villinger & Grevemeyer, 2001
1841.502	1.190376	Villinger & Grevemeyer, 2001
1841.277	1.194887	Villinger & Grevemeyer, 2001
1841.277	1.200602	Villinger & Grevemeyer, 2001
1843.975	1.204511	Villinger & Grevemeyer, 2001
1847.797	1.20782	Villinger & Grevemeyer, 2001
1850.495	1.210526	Villinger & Grevemeyer, 2001
1852.068	1.206617	Villinger & Grevemeyer, 2001
1851.169	1.196993	Villinger & Grevemeyer, 2001
1854.092	1.198196	Villinger & Grevemeyer, 2001
1856.115	1.199098	Villinger & Grevemeyer, 2001
1854.991	1.194587	Villinger & Grevemeyer, 2001
1854.541	1.189774	Villinger & Grevemeyer, 2001
1854.541	1.186466	Villinger & Grevemeyer, 2001
1834.982	1.216541	Villinger & Grevemeyer, 2001
1823.966	1.224361	Villinger & Grevemeyer, 2001
1823.067	1.225865	Villinger & Grevemeyer, 2001
1821.718	1.229173	Villinger & Grevemeyer, 2001

1821.268	1.234587	Villinger & Grevemeyer, 2001
1823.067	1.241504	Villinger & Grevemeyer, 2001
1820.594	1.252331	Villinger & Grevemeyer, 2001
1826.439	1.249624	Villinger & Grevemeyer, 2001
1827.563	1.246015	Villinger & Grevemeyer, 2001
1829.586	1.243609	Villinger & Grevemeyer, 2001
1829.137	1.239699	Villinger & Grevemeyer, 2001
1826.439	1.236692	Villinger & Grevemeyer, 2001
1827.113	1.230977	Villinger & Grevemeyer, 2001
1830.261	1.230677	Villinger & Grevemeyer, 2001
1832.959	1.233083	Villinger & Grevemeyer, 2001
1836.556	1.231579	Villinger & Grevemeyer, 2001
1837.905	1.230075	Villinger & Grevemeyer, 2001
1839.928	1.223158	Villinger & Grevemeyer, 2001
1842.626	1.219248	Villinger & Grevemeyer, 2001
1825.989	1.257444	Villinger & Grevemeyer, 2001
1830.935	1.259248	Villinger & Grevemeyer, 2001
1834.083	1.255038	Villinger & Grevemeyer, 2001
1828.912	1.262857	Villinger & Grevemeyer, 2001
1834.308	1.258647	Villinger & Grevemeyer, 2001
1837.68	1.258647	Villinger & Grevemeyer, 2001
1834.982	1.282406	Villinger & Grevemeyer, 2001
1837.005	1.283308	Villinger & Grevemeyer, 2001
1834.982	1.273384	Villinger & Grevemeyer, 2001
1839.254	1.27218	Villinger & Grevemeyer, 2001
1840.827	1.270376	Villinger & Grevemeyer, 2001
1843.3	1.26797	Villinger & Grevemeyer, 2001
1844.649	1.26797	Villinger & Grevemeyer, 2001
1846.673	1.277895	Villinger & Grevemeyer, 2001

1851.394	1.279398	Villinger & Grevemeyer, 2001
1851.394	1.27188	Villinger & Grevemeyer, 2001
1856.34	1.271579	Villinger & Grevemeyer, 2001
1858.363	1.269173	Villinger & Grevemeyer, 2001
1857.689	1.280902	Villinger & Grevemeyer, 2001
1860.162	1.27609	Villinger & Grevemeyer, 2001
1863.309	1.273985	Villinger & Grevemeyer, 2001
1848.471	1.257744	Villinger & Grevemeyer, 2001
1855.665	1.260752	Villinger & Grevemeyer, 2001
1860.387	1.25594	Villinger & Grevemeyer, 2001
1863.534	1.256842	Villinger & Grevemeyer, 2001
1868.255	1.265865	Villinger & Grevemeyer, 2001
1868.705	1.260451	Villinger & Grevemeyer, 2001
1872.527	1.261654	Villinger & Grevemeyer, 2001
1881.52	1.275188	Villinger & Grevemeyer, 2001
1888.489	1.274286	Villinger & Grevemeyer, 2001
1888.04	1.277594	Villinger & Grevemeyer, 2001
1895.459	1.281504	Villinger & Grevemeyer, 2001
1899.281	1.277895	Villinger & Grevemeyer, 2001
1902.878	1.276391	Villinger & Grevemeyer, 2001
1906.025	1.27218	Villinger & Grevemeyer, 2001
1908.498	1.271278	Villinger & Grevemeyer, 2001
1903.777	1.269774	Villinger & Grevemeyer, 2001
1899.955	1.270376	Villinger & Grevemeyer, 2001
1897.932	1.27188	Villinger & Grevemeyer, 2001
1941.097	1.278196	Villinger & Grevemeyer, 2001
1942.446	1.27609	Villinger & Grevemeyer, 2001
1941.547	1.270075	Villinger & Grevemeyer, 2001
1939.973	1.267368	Villinger & Grevemeyer, 2001

1939.299	1.27188	Villinger & Grevemeyer, 2001
1936.151	1.273083	Villinger & Grevemeyer, 2001
1935.702	1.270075	Villinger & Grevemeyer, 2001
1935.477	1.267368	Villinger & Grevemeyer, 2001
1931.205	1.270376	Villinger & Grevemeyer, 2001
1928.282	1.267669	Villinger & Grevemeyer, 2001
1931.205	1.266165	Villinger & Grevemeyer, 2001
1932.554	1.263759	Villinger & Grevemeyer, 2001
1930.306	1.261353	Villinger & Grevemeyer, 2001
1927.158	1.26015	Villinger & Grevemeyer, 2001
1924.91	1.260451	Villinger & Grevemeyer, 2001
1927.833	1.25594	Villinger & Grevemeyer, 2001
1928.282	1.253534	Villinger & Grevemeyer, 2001
1912.095	1.262556	Villinger & Grevemeyer, 2001
1912.77	1.26015	Villinger & Grevemeyer, 2001
1915.468	1.255038	Villinger & Grevemeyer, 2001
1920.638	1.255038	Villinger & Grevemeyer, 2001
1921.313	1.250226	Villinger & Grevemeyer, 2001
1923.786	1.243308	Villinger & Grevemeyer, 2001
1925.585	1.24	Villinger & Grevemeyer, 2001
1920.189	1.245714	Villinger & Grevemeyer, 2001
1917.041	1.246015	Villinger & Grevemeyer, 2001
1914.568	1.249925	Villinger & Grevemeyer, 2001
1911.421	1.249323	Villinger & Grevemeyer, 2001
1909.398	1.252331	Villinger & Grevemeyer, 2001
1906.475	1.254737	Villinger & Grevemeyer, 2001
1904.227	1.251729	Villinger & Grevemeyer, 2001
1902.203	1.247519	Villinger & Grevemeyer, 2001
1906.925	1.245113	Villinger & Grevemeyer, 2001

1912.095	1.242105	Villinger & Grevemeyer, 2001
1914.119	1.238196	Villinger & Grevemeyer, 2001
1916.592	1.238496	Villinger & Grevemeyer, 2001
1919.514	1.238496	Villinger & Grevemeyer, 2001
1919.29	1.232782	Villinger & Grevemeyer, 2001
1916.817	1.233684	Villinger & Grevemeyer, 2001
1895.009	1.262857	Villinger & Grevemeyer, 2001
1897.257	1.251729	Villinger & Grevemeyer, 2001
1903.327	1.239399	Villinger & Grevemeyer, 2001
1901.529	1.237293	Villinger & Grevemeyer, 2001
1901.978	1.232481	Villinger & Grevemeyer, 2001
1903.552	1.227369	Villinger & Grevemeyer, 2001
1906.025	1.231579	Villinger & Grevemeyer, 2001
1906.925	1.225564	Villinger & Grevemeyer, 2001
1909.847	1.226165	Villinger & Grevemeyer, 2001
1909.398	1.233383	Villinger & Grevemeyer, 2001
1890.513	1.253233	Villinger & Grevemeyer, 2001
1889.388	1.24812	Villinger & Grevemeyer, 2001
1892.536	1.24812	Villinger & Grevemeyer, 2001
1895.009	1.247519	Villinger & Grevemeyer, 2001
1897.032	1.241504	Villinger & Grevemeyer, 2001
1895.009	1.243008	Villinger & Grevemeyer, 2001
1893.435	1.240902	Villinger & Grevemeyer, 2001
1888.939	1.243308	Villinger & Grevemeyer, 2001
1886.016	1.242707	Villinger & Grevemeyer, 2001
1887.59	1.242105	Villinger & Grevemeyer, 2001
1886.466	1.238196	Villinger & Grevemeyer, 2001
1882.869	1.239699	Villinger & Grevemeyer, 2001
1880.396	1.240602	Villinger & Grevemeyer, 2001

1879.497	1.244511	Villinger & Grevemeyer, 2001
1880.845	1.247218	Villinger & Grevemeyer, 2001
1883.318	1.248722	Villinger & Grevemeyer, 2001
1879.047	1.251429	Villinger & Grevemeyer, 2001
1878.597	1.255338	Villinger & Grevemeyer, 2001
1877.023	1.24782	Villinger & Grevemeyer, 2001
1876.124	1.244211	Villinger & Grevemeyer, 2001
1873.202	1.243308	Villinger & Grevemeyer, 2001
1872.752	1.247218	Villinger & Grevemeyer, 2001
1870.953	1.247218	Villinger & Grevemeyer, 2001
1870.504	1.244812	Villinger & Grevemeyer, 2001
1866.682	1.246917	Villinger & Grevemeyer, 2001
1865.108	1.248421	Villinger & Grevemeyer, 2001
1868.255	1.251128	Villinger & Grevemeyer, 2001
1869.38	1.253534	Villinger & Grevemeyer, 2001
1876.349	1.237293	Villinger & Grevemeyer, 2001
1880.396	1.235789	Villinger & Grevemeyer, 2001
1878.148	1.23188	Villinger & Grevemeyer, 2001
1877.023	1.232782	Villinger & Grevemeyer, 2001
1875.45	1.231579	Villinger & Grevemeyer, 2001
1874.101	1.229474	Villinger & Grevemeyer, 2001
1869.829	1.233985	Villinger & Grevemeyer, 2001
1866.907	1.235789	Villinger & Grevemeyer, 2001
1866.907	1.238797	Villinger & Grevemeyer, 2001
1865.558	1.240602	Villinger & Grevemeyer, 2001
1863.309	1.241805	Villinger & Grevemeyer, 2001
1861.511	1.245113	Villinger & Grevemeyer, 2001
1856.34	1.244511	Villinger & Grevemeyer, 2001
1853.192	1.24782	Villinger & Grevemeyer, 2001

1859.937	1.237895	Villinger & Grevemeyer, 2001
1861.736	1.232181	Villinger & Grevemeyer, 2001
1864.658	1.230376	Villinger & Grevemeyer, 2001
1862.635	1.222256	Villinger & Grevemeyer, 2001
1857.239	1.224662	Villinger & Grevemeyer, 2001
1859.487	1.229474	Villinger & Grevemeyer, 2001
1857.914	1.233083	Villinger & Grevemeyer, 2001
1856.34	1.229474	Villinger & Grevemeyer, 2001
1853.867	1.23188	Villinger & Grevemeyer, 2001
1850.944	1.227669	Villinger & Grevemeyer, 2001
1849.82	1.232481	Villinger & Grevemeyer, 2001
1846.898	1.223158	Villinger & Grevemeyer, 2001
1845.773	1.230376	Villinger & Grevemeyer, 2001
1843.75	1.232782	Villinger & Grevemeyer, 2001
1841.277	1.234887	Villinger & Grevemeyer, 2001
1838.579	1.236692	Villinger & Grevemeyer, 2001
1837.455	1.239098	Villinger & Grevemeyer, 2001
1836.331	1.242707	Villinger & Grevemeyer, 2001
1837.68	1.246015	Villinger & Grevemeyer, 2001
1841.502	1.247218	Villinger & Grevemeyer, 2001
1842.176	1.250827	Villinger & Grevemeyer, 2001
1841.727	1.252932	Villinger & Grevemeyer, 2001
1841.277	1.242105	Villinger & Grevemeyer, 2001
1842.851	1.240301	Villinger & Grevemeyer, 2001
1846.223	1.243308	Villinger & Grevemeyer, 2001
1847.122	1.244812	Villinger & Grevemeyer, 2001
1846.673	1.237895	Villinger & Grevemeyer, 2001
1848.022	1.234286	Villinger & Grevemeyer, 2001
1856.34	1.211429	Villinger & Grevemeyer, 2001

1860.836	1.214436	Villinger & Grevemeyer, 2001
1859.712	1.205714	Villinger & Grevemeyer, 2001
1862.86	1.208421	Villinger & Grevemeyer, 2001
1857.689	1.182256	Villinger & Grevemeyer, 2001
1860.162	1.179248	Villinger & Grevemeyer, 2001
1862.41	1.194286	Villinger & Grevemeyer, 2001
1863.984	1.198496	Villinger & Grevemeyer, 2001
1863.534	1.187669	Villinger & Grevemeyer, 2001
1865.558	1.205113	Villinger & Grevemeyer, 2001
1868.705	1.213534	Villinger & Grevemeyer, 2001
1874.326	1.219248	Villinger & Grevemeyer, 2001
1871.403	1.205714	Villinger & Grevemeyer, 2001
1868.48	1.196391	Villinger & Grevemeyer, 2001
1872.752	1.198496	Villinger & Grevemeyer, 2001
1868.705	1.184962	Villinger & Grevemeyer, 2001
1864.209	1.173233	Villinger & Grevemeyer, 2001
1872.077	1.152782	Villinger & Grevemeyer, 2001
1875.675	1.178346	Villinger & Grevemeyer, 2001
1876.799	1.184662	Villinger & Grevemeyer, 2001
1874.775	1.187368	Villinger & Grevemeyer, 2001
1876.124	1.192782	Villinger & Grevemeyer, 2001
1877.473	1.198496	Villinger & Grevemeyer, 2001
1875	1.195489	Villinger & Grevemeyer, 2001
1881.295	1.19188	Villinger & Grevemeyer, 2001
1878.822	1.182857	Villinger & Grevemeyer, 2001
1878.597	1.179248	Villinger & Grevemeyer, 2001
1881.52	1.176842	Villinger & Grevemeyer, 2001
1883.094	1.17594	Villinger & Grevemeyer, 2001
1884.667	1.179549	Villinger & Grevemeyer, 2001

1886.241	1.182256	Villinger & Grevemeyer, 2001
1884.667	1.153384	Villinger & Grevemeyer, 2001
1894.784	1.151278	Villinger & Grevemeyer, 2001
1908.049	1.149173	Villinger & Grevemeyer, 2001
1920.863	1.160602	Villinger & Grevemeyer, 2001
1904.901	1.172932	Villinger & Grevemeyer, 2001
1910.747	1.172632	Villinger & Grevemeyer, 2001
1902.653	1.178045	Villinger & Grevemeyer, 2001
1908.273	1.180451	Villinger & Grevemeyer, 2001
1905.126	1.186166	Villinger & Grevemeyer, 2001
1901.754	1.185865	Villinger & Grevemeyer, 2001
1902.428	1.196692	Villinger & Grevemeyer, 2001
1899.955	1.190978	Villinger & Grevemeyer, 2001
1897.707	1.193684	Villinger & Grevemeyer, 2001
1897.257	1.196692	Villinger & Grevemeyer, 2001
1893.21	1.189774	Villinger & Grevemeyer, 2001
1889.164	1.189173	Villinger & Grevemeyer, 2001
1891.187	1.196993	Villinger & Grevemeyer, 2001
1886.466	1.192782	Villinger & Grevemeyer, 2001
1885.117	1.194286	Villinger & Grevemeyer, 2001
1885.117	1.199399	Villinger & Grevemeyer, 2001
1883.768	1.203008	Villinger & Grevemeyer, 2001
1880.845	1.209023	Villinger & Grevemeyer, 2001
1882.194	1.209925	Villinger & Grevemeyer, 2001
1886.466	1.206316	Villinger & Grevemeyer, 2001
1889.164	1.207519	Villinger & Grevemeyer, 2001
1891.187	1.208722	Villinger & Grevemeyer, 2001
1892.986	1.204511	Villinger & Grevemeyer, 2001
1895.908	1.206316	Villinger & Grevemeyer, 2001

1898.606	1.205414	Villinger & Grevemeyer, 2001
1901.079	1.205414	Villinger & Grevemeyer, 2001
1905.126	1.207519	Villinger & Grevemeyer, 2001
1880.171	1.227369	Villinger & Grevemeyer, 2001
1881.745	1.225263	Villinger & Grevemeyer, 2001
1883.768	1.227068	Villinger & Grevemeyer, 2001
1886.016	1.230977	Villinger & Grevemeyer, 2001
1888.489	1.233383	Villinger & Grevemeyer, 2001
1891.637	1.234587	Villinger & Grevemeyer, 2001
1894.335	1.233985	Villinger & Grevemeyer, 2001
1896.133	1.230677	Villinger & Grevemeyer, 2001
1898.381	1.227369	Villinger & Grevemeyer, 2001
1898.381	1.225263	Villinger & Grevemeyer, 2001
1896.358	1.223459	Villinger & Grevemeyer, 2001
1893.66	1.222556	Villinger & Grevemeyer, 2001
1891.412	1.223158	Villinger & Grevemeyer, 2001
1890.063	1.224962	Villinger & Grevemeyer, 2001
1911.196	1.218947	Villinger & Grevemeyer, 2001
1912.995	1.221353	Villinger & Grevemeyer, 2001
1915.917	1.223158	Villinger & Grevemeyer, 2001
1911.646	1.208722	Villinger & Grevemeyer, 2001
1909.622	1.197293	Villinger & Grevemeyer, 2001
1911.421	1.195188	Villinger & Grevemeyer, 2001
1915.018	1.194286	Villinger & Grevemeyer, 2001
1917.041	1.196692	Villinger & Grevemeyer, 2001
1914.344	1.199699	Villinger & Grevemeyer, 2001
1917.716	1.203308	Villinger & Grevemeyer, 2001
1919.065	1.2	Villinger & Grevemeyer, 2001
1921.313	1.199699	Villinger & Grevemeyer, 2001

1923.786	1.204812	Villinger & Grevemeyer, 2001
1912.32	1.187068	Villinger & Grevemeyer, 2001
1913.669	1.184361	Villinger & Grevemeyer, 2001
1913.894	1.174436	Villinger & Grevemeyer, 2001
1914.344	1.181053	Villinger & Grevemeyer, 2001
1920.863	1.187368	Villinger & Grevemeyer, 2001
1922.437	1.180752	Villinger & Grevemeyer, 2001
1920.638	1.176541	Villinger & Grevemeyer, 2001
1923.336	1.171128	Villinger & Grevemeyer, 2001
1925.585	1.176541	Villinger & Grevemeyer, 2001
1928.507	1.170526	Villinger & Grevemeyer, 2001
1937.275	1.176842	Villinger & Grevemeyer, 2001
1954.362	1.177744	Villinger & Grevemeyer, 2001
1940.198	1.182256	Villinger & Grevemeyer, 2001
1935.027	1.184962	Villinger & Grevemeyer, 2001
1928.282	1.189173	Villinger & Grevemeyer, 2001
1926.034	1.19188	Villinger & Grevemeyer, 2001
1927.158	1.197594	Villinger & Grevemeyer, 2001
1929.856	1.194587	Villinger & Grevemeyer, 2001
1930.98	1.191579	Villinger & Grevemeyer, 2001
1932.329	1.199399	Villinger & Grevemeyer, 2001
1937.05	1.201805	Villinger & Grevemeyer, 2001
1937.275	1.198196	Villinger & Grevemeyer, 2001
1937.05	1.194587	Villinger & Grevemeyer, 2001
1938.175	1.19218	Villinger & Grevemeyer, 2001
1944.47	1.186767	Villinger & Grevemeyer, 2001
1944.02	1.19188	Villinger & Grevemeyer, 2001
1946.718	1.189774	Villinger & Grevemeyer, 2001
1956.16	1.187368	Villinger & Grevemeyer, 2001

1957.284	1.189774	Villinger & Grevemeyer, 2001
1959.532	1.191579	Villinger & Grevemeyer, 2001
1955.935	1.194887	Villinger & Grevemeyer, 2001
1950.989	1.196993	Villinger & Grevemeyer, 2001
1954.811	1.201504	Villinger & Grevemeyer, 2001
1958.183	1.196692	Villinger & Grevemeyer, 2001
1957.734	1.204511	Villinger & Grevemeyer, 2001
1960.657	1.204812	Villinger & Grevemeyer, 2001
1962.68	1.201203	Villinger & Grevemeyer, 2001
1965.153	1.2	Villinger & Grevemeyer, 2001
1967.851	1.197594	Villinger & Grevemeyer, 2001
1969.649	1.195188	Villinger & Grevemeyer, 2001
1941.097	1.199098	Villinger & Grevemeyer, 2001
1942.896	1.200902	Villinger & Grevemeyer, 2001
1946.043	1.2	Villinger & Grevemeyer, 2001
1946.718	1.202707	Villinger & Grevemeyer, 2001
1947.617	1.205714	Villinger & Grevemeyer, 2001
1948.741	1.20782	Villinger & Grevemeyer, 2001
1951.439	1.209624	Villinger & Grevemeyer, 2001
1952.788	1.206015	Villinger & Grevemeyer, 2001
1956.61	1.212331	Villinger & Grevemeyer, 2001
1954.362	1.212932	Villinger & Grevemeyer, 2001
1953.013	1.216241	Villinger & Grevemeyer, 2001
1940.648	1.206015	Villinger & Grevemeyer, 2001
1943.795	1.210827	Villinger & Grevemeyer, 2001
1944.245	1.213835	Villinger & Grevemeyer, 2001
1943.121	1.217143	Villinger & Grevemeyer, 2001
1940.648	1.211729	Villinger & Grevemeyer, 2001
1938.849	1.209925	Villinger & Grevemeyer, 2001

1936.601	1.211128	Villinger & Grevemeyer, 2001
1933.453	1.206015	Villinger & Grevemeyer, 2001
1930.755	1.207218	Villinger & Grevemeyer, 2001
1933.678	1.215338	Villinger & Grevemeyer, 2001
1929.182	1.214737	Villinger & Grevemeyer, 2001
1927.158	1.21594	Villinger & Grevemeyer, 2001
1923.561	1.216842	Villinger & Grevemeyer, 2001
1922.887	1.212932	Villinger & Grevemeyer, 2001
1917.716	1.211729	Villinger & Grevemeyer, 2001
1918.165	1.216241	Villinger & Grevemeyer, 2001
1926.709	1.223158	Villinger & Grevemeyer, 2001
1923.786	1.226165	Villinger & Grevemeyer, 2001
1927.383	1.232181	Villinger & Grevemeyer, 2001
1933.228	1.229775	Villinger & Grevemeyer, 2001
1935.252	1.226466	Villinger & Grevemeyer, 2001
1938.624	1.225865	Villinger & Grevemeyer, 2001
1940.648	1.22797	Villinger & Grevemeyer, 2001
1937.725	1.227068	Villinger & Grevemeyer, 2001
1944.245	1.225564	Villinger & Grevemeyer, 2001
1941.997	1.229173	Villinger & Grevemeyer, 2001
1944.02	1.233985	Villinger & Grevemeyer, 2001
1931.205	1.24	Villinger & Grevemeyer, 2001
1931.655	1.24391	Villinger & Grevemeyer, 2001
1932.329	1.245113	Villinger & Grevemeyer, 2001
1933.004	1.247519	Villinger & Grevemeyer, 2001
1932.329	1.249624	Villinger & Grevemeyer, 2001
1935.027	1.25203	Villinger & Grevemeyer, 2001
1935.027	1.253835	Villinger & Grevemeyer, 2001
1935.926	1.256241	Villinger & Grevemeyer, 2001

1937.5	1.257444	Villinger & Grevemeyer, 2001
1939.074	1.258346	Villinger & Grevemeyer, 2001
1942.896	1.260752	Villinger & Grevemeyer, 2001
1946.043	1.264361	Villinger & Grevemeyer, 2001
1947.167	1.265564	Villinger & Grevemeyer, 2001
1950.09	1.269474	Villinger & Grevemeyer, 2001
1939.074	1.248421	Villinger & Grevemeyer, 2001
1940.423	1.250827	Villinger & Grevemeyer, 2001
1941.097	1.252632	Villinger & Grevemeyer, 2001
1942.221	1.253835	Villinger & Grevemeyer, 2001
1943.345	1.254737	Villinger & Grevemeyer, 2001
1945.369	1.258045	Villinger & Grevemeyer, 2001
1943.345	1.245714	Villinger & Grevemeyer, 2001
1945.144	1.243609	Villinger & Grevemeyer, 2001
1946.718	1.242707	Villinger & Grevemeyer, 2001
1947.617	1.245714	Villinger & Grevemeyer, 2001
1946.718	1.24782	Villinger & Grevemeyer, 2001
1947.617	1.251128	Villinger & Grevemeyer, 2001
1948.516	1.253835	Villinger & Grevemeyer, 2001
1950.315	1.249925	Villinger & Grevemeyer, 2001
1951.664	1.249323	Villinger & Grevemeyer, 2001
1951.214	1.253534	Villinger & Grevemeyer, 2001
1951.214	1.257444	Villinger & Grevemeyer, 2001
1951.439	1.260451	Villinger & Grevemeyer, 2001
1951.888	1.263158	Villinger & Grevemeyer, 2001
1954.811	1.266767	Villinger & Grevemeyer, 2001
1955.036	1.251729	Villinger & Grevemeyer, 2001
1955.036	1.24812	Villinger & Grevemeyer, 2001
1956.61	1.24391	Villinger & Grevemeyer, 2001

1958.408	1.249023	Villinger & Grevemeyer, 2001
1960.432	1.252331	Villinger & Grevemeyer, 2001
1962.005	1.253233	Villinger & Grevemeyer, 2001
1963.354	1.254436	Villinger & Grevemeyer, 2001
1958.633	1.258947	Villinger & Grevemeyer, 2001
1958.183	1.26015	Villinger & Grevemeyer, 2001
1956.61	1.268872	Villinger & Grevemeyer, 2001
1959.757	1.277293	Villinger & Grevemeyer, 2001
1964.703	1.280602	Villinger & Grevemeyer, 2001
1967.176	1.277594	Villinger & Grevemeyer, 2001
1968.076	1.275489	Villinger & Grevemeyer, 2001
1962.005	1.271579	Villinger & Grevemeyer, 2001
1962.23	1.26797	Villinger & Grevemeyer, 2001
1963.804	1.265564	Villinger & Grevemeyer, 2001
1965.153	1.263759	Villinger & Grevemeyer, 2001
1969.425	1.260752	Villinger & Grevemeyer, 2001
1970.099	1.264962	Villinger & Grevemeyer, 2001
1968.975	1.267669	Villinger & Grevemeyer, 2001
1970.998	1.270978	Villinger & Grevemeyer, 2001
1973.471	1.27579	Villinger & Grevemeyer, 2001
1975.27	1.277895	Villinger & Grevemeyer, 2001
1979.317	1.272782	Villinger & Grevemeyer, 2001
1977.743	1.270677	Villinger & Grevemeyer, 2001
1976.844	1.268271	Villinger & Grevemeyer, 2001
1975.27	1.267068	Villinger & Grevemeyer, 2001
1974.146	1.264361	Villinger & Grevemeyer, 2001
1972.347	1.262857	Villinger & Grevemeyer, 2001
1973.247	1.259549	Villinger & Grevemeyer, 2001
1974.371	1.257444	Villinger & Grevemeyer, 2001

1975.944	1.257143	Villinger & Grevemeyer, 2001
1978.192	1.259549	Villinger & Grevemeyer, 2001
1977.293	1.226466	Villinger & Grevemeyer, 2001
1979.092	1.253233	Villinger & Grevemeyer, 2001
1979.541	1.250226	Villinger & Grevemeyer, 2001
1981.565	1.242105	Villinger & Grevemeyer, 2001
1978.417	1.245113	Villinger & Grevemeyer, 2001
1975.72	1.245113	Villinger & Grevemeyer, 2001
1978.867	1.24	Villinger & Grevemeyer, 2001
1978.642	1.23609	Villinger & Grevemeyer, 2001
1977.518	1.231579	Villinger & Grevemeyer, 2001
1977.293	1.222256	Villinger & Grevemeyer, 2001
1978.867	1.21203	Villinger & Grevemeyer, 2001
1976.619	1.212932	Villinger & Grevemeyer, 2001
1974.146	1.212632	Villinger & Grevemeyer, 2001
1972.797	1.210827	Villinger & Grevemeyer, 2001
1972.797	1.218346	Villinger & Grevemeyer, 2001
1971.448	1.219248	Villinger & Grevemeyer, 2001
1972.347	1.24	Villinger & Grevemeyer, 2001
1974.595	1.233985	Villinger & Grevemeyer, 2001
1974.146	1.238496	Villinger & Grevemeyer, 2001
1970.773	1.243609	Villinger & Grevemeyer, 2001
1968.3	1.245113	Villinger & Grevemeyer, 2001
1969.2	1.251429	Villinger & Grevemeyer, 2001
1967.176	1.255338	Villinger & Grevemeyer, 2001
1968.975	1.233383	Villinger & Grevemeyer, 2001
1968.975	1.214436	Villinger & Grevemeyer, 2001
1963.804	1.246617	Villinger & Grevemeyer, 2001
1965.153	1.222256	Villinger & Grevemeyer, 2001

1964.928	1.216241	Villinger & Grevemeyer, 2001
1962.005	1.211128	Villinger & Grevemeyer, 2001
1962.005	1.217444	Villinger & Grevemeyer, 2001
1960.657	1.227068	Villinger & Grevemeyer, 2001
1962.68	1.232782	Villinger & Grevemeyer, 2001
1963.804	1.235188	Villinger & Grevemeyer, 2001
1959.083	1.239399	Villinger & Grevemeyer, 2001
1958.633	1.234887	Villinger & Grevemeyer, 2001
1954.137	1.228571	Villinger & Grevemeyer, 2001
1955.261	1.236391	Villinger & Grevemeyer, 2001
1951.214	1.234286	Villinger & Grevemeyer, 2001
1950.764	1.238496	Villinger & Grevemeyer, 2001
1949.64	1.239699	Villinger & Grevemeyer, 2001
5812.05	3.34603	Hartmann et al., 2005
5313.9	3.30901	Hartmann et al., 2005
4612.25	3.41496	Hartmann et al., 2005
4352.72	3.16761	Hartmann et al., 2005
4536.56	3.00313	Hartmann et al., 2005
4288.62	2.69385	Hartmann et al., 2005
4179.55	2.94977	Hartmann et al., 2005
4148	2.88789	Hartmann et al., 2005
3994.96	2.85579	Hartmann et al., 2005
3850.32	3.01483	Hartmann et al., 2005
3767.49	2.84801	Hartmann et al., 2005
3841.82	2.7833	Hartmann et al., 2005
3775.05	2.74839	Hartmann et al., 2005
3676.85	2.69198	Hartmann et al., 2005
3555.48	2.76215	Hartmann et al., 2005
3425.85	2.68694	Hartmann et al., 2005

3076.57	2.59317	Hartmann et al., 2005
3119.83	2.63619	Hartmann et al., 2005
3170.82	2.64151	Hartmann et al., 2005
3202.24	2.65762	Hartmann et al., 2005
3112.45	2.80043	Hartmann et al., 2005
3163.26	2.74113	Hartmann et al., 2005
3202.4	2.71416	Hartmann et al., 2005
3225.79	2.66567	Hartmann et al., 2005
3308.28	2.71132	Hartmann et al., 2005
3312.36	2.76786	Hartmann et al., 2005
3249.85	2.84871	Hartmann et al., 2005
3226.62	2.95374	Hartmann et al., 2005
3269.82	2.97792	Hartmann et al., 2005
3371.46	2.8647	Hartmann et al., 2005
3367.61	2.88894	Hartmann et al., 2005
3441.87	2.80268	Hartmann et al., 2005
3560.1	3.00714	Hartmann et al., 2005
3352.74	3.17434	Hartmann et al., 2005
5330.6	3.66168	Hartmann et al., 2005
5252.13	3.64833	Hartmann et al., 2005
4400.5	3.42063	Hartmann et al., 2005
4298.28	3.32922	Hartmann et al., 2005
4513.8	3.2724	Hartmann et al., 2005
4004.11	3.31077	Hartmann et al., 2005
3847.48	3.39445	Hartmann et al., 2005
3780.75	3.37031	Hartmann et al., 2005
3749.06	3.25996	Hartmann et al., 2005
3890.23	3.25977	Hartmann et al., 2005
3952.48	3.08469	Hartmann et al., 2005

3924.88	3.03357	Hartmann et al., 2005
3897.43	3.03361	Hartmann et al., 2005
3803.58	3.12527	Hartmann et al., 2005
3784.08	3.16299	Hartmann et al., 2005
3678.44	3.24929	Hartmann et al., 2005
3788.31	3.27337	Hartmann et al., 2005
3412.22	3.4058	Hartmann et al., 2005
3572.47	3.21982	Hartmann et al., 2005
3552.8	3.19561	Hartmann et al., 2005
3544.82	3.14716	Hartmann et al., 2005
3654.54	3.12009	Hartmann et al., 2005
3701.43	3.0608	Hartmann et al., 2005
3744.68	3.09843	Hartmann et al., 2005
3650.15	2.95586	Hartmann et al., 2005
3685.72	3.05274	Hartmann et al., 2005
3556.23	3.02599	Hartmann et al., 2005
3524.71	2.97219	Hartmann et al., 2005
3489.38	2.96147	Hartmann et al., 2005
3473.58	2.9211	Hartmann et al., 2005
3473.45	2.87533	Hartmann et al., 2005
3422.59	2.91579	Hartmann et al., 2005
3194.23	2.5984	Hartmann et al., 2005
2787.24	2.8978	Hartmann et al., 2005
2932.27	2.87337	Hartmann et al., 2005
3089.04	2.84085	Hartmann et al., 2005
3257.77	2.87562	Hartmann et al., 2005
3018.72	2.93518	Hartmann et al., 2005
3065.68	2.90011	Hartmann et al., 2005
3136.32	2.91886	Hartmann et al., 2005

3120.57	2.89735	Hartmann et al., 2005
3266.22	3.091	Hartmann et al., 2005
2995.27	2.96213	Hartmann et al., 2005
2924.67	2.95953	Hartmann et al., 2005
2928.47	2.91645	Hartmann et al., 2005
2959.85	2.9191	Hartmann et al., 2005
3014.71	2.90287	Hartmann et al., 2005
3163.88	2.95652	Hartmann et al., 2005
3238.4	2.9618	Hartmann et al., 2005
3293.38	2.98865	Hartmann et al., 2005
3215	3.0076	Hartmann et al., 2005
3152.31	3.02654	Hartmann et al., 2005
3121.04	3.06158	Hartmann et al., 2005
3074.01	3.07241	Hartmann et al., 2005
3030.76	3.03208	Hartmann et al., 2005
2952.25	3.00527	Hartmann et al., 2005
2999.32	3.0079	Hartmann et al., 2005
2983.75	3.0483	Hartmann et al., 2005
3081.74	3.03202	Hartmann et al., 2005
2921.02	3.05377	Hartmann et al., 2005
3042.8	3.12899	Hartmann et al., 2005
3215.43	3.15568	Hartmann et al., 2005
3321.55	3.239	Hartmann et al., 2005
3376.61	3.29547	Hartmann et al., 2005
3462.62	3.20112	Hartmann et al., 2005
3380.2	3.17969	Hartmann et al., 2005
3434.96	3.12846	Hartmann et al., 2005
3481.9	3.08802	Hartmann et al., 2005
3415.1	3.03964	Hartmann et al., 2005

3344.66	3.09358	Hartmann et al., 2005
3317.33	3.1367	Hartmann et al., 2005
3191.71	3.08841	Hartmann et al., 2005
3199.42	3.04263	Hartmann et al., 2005
3124.76	2.98888	Hartmann et al., 2005
3297.49	3.05326	Hartmann et al., 2005
3348.41	3.03435	Hartmann et al., 2005
3336.54	2.99667	Hartmann et al., 2005
3293.27	2.94827	Hartmann et al., 2005
3379.62	2.97508	Hartmann et al., 2005
3415.01	3.01003	Hartmann et al., 2005
3065.92	2.98627	Hartmann et al., 2005
3081.53	2.95932	Hartmann et al., 2005
3053.84	2.8759	Hartmann et al., 2005
3128.17	2.81118	Hartmann et al., 2005
2877.57	2.94614	Hartmann et al., 2005
3438.4	2.96153	Hartmann et al., 2005
3571.72	2.95597	Hartmann et al., 2005
3415.26	3.09618	Hartmann et al., 2005
3654.76	3.19817	Hartmann et al., 2005
3674.25	3.15506	Hartmann et al., 2005
3740.89	3.14421	Hartmann et al., 2005
2658.89	2.10932	Gu et al., 2017
2592.17	2.12007	Gu et al., 2017
2630.9	2.17757	Gu et al., 2017
2649.89	2.20364	Gu et al., 2017
2663.51	2.18021	Gu et al., 2017
2734.1	2.23969	Gu et al., 2017
2589.99	2.21171	Gu et al., 2017

2465.62	2.20379	Gu et al., 2017
2440.64	2.24261	Gu et al., 2017
2458.11	2.26868	Gu et al., 2017
2539.25	2.26995	Gu et al., 2017
2565.78	2.25856	Gu et al., 2017
2577.94	2.28396	Gu et al., 2017
2467.25	2.3068	Gu et al., 2017
2515.07	2.35224	Gu et al., 2017
2578.11	2.44249	Gu et al., 2017
2643.31	2.43174	Gu et al., 2017
2636.56	2.50264	Gu et al., 2017
2733.56	2.44972	Gu et al., 2017
2808.61	2.42692	Gu et al., 2017
2867.05	2.47369	Gu et al., 2017
2835.24	2.50649	Gu et al., 2017
2848.13	2.5125	Gu et al., 2017
2842.09	2.53659	Gu et al., 2017
2831.49	2.54529	Gu et al., 2017
2757.91	2.52796	Gu et al., 2017
2790.56	2.56472	Gu et al., 2017
2745.81	2.55807	Gu et al., 2017
2725.35	2.56612	Gu et al., 2017
2741.3	2.59486	Gu et al., 2017
2783.02	2.60353	Gu et al., 2017
4651	3.31	Jorand et al., 2015
4930	3.31	Jorand et al., 2015
4325	4.38	Jorand et al., 2015
4244	4.51	Jorand et al., 2015
5029	3.37	Jorand et al., 2015

4796	3.52	Jorand et al., 2015
5298	4.46	Jorand et al., 2015
5869	3.35	Jorand et al., 2015
5998	3.35	Jorand et al., 2015
5597	2.9	Jorand et al., 2015
3035	2.72	Esteban et al., 2015
2062	2.88	Esteban et al., 2015
2851	3.6	Esteban et al., 2015
2653	3.59	Esteban et al., 2015
2754	4.2	Esteban et al., 2015
3225	4.31	Esteban et al., 2015
3358	4.01	Esteban et al., 2015
2965	4.22	Esteban et al., 2015
2801	4.13	Esteban et al., 2015
3052	4.96	Esteban et al., 2015
3042	4.89	Esteban et al., 2015
3144	4.32	Esteban et al., 2015
3446	4.43	Esteban et al., 2015
3232	4.25	Esteban et al., 2015
2904	4.6	Esteban et al., 2015
3063	4.08	Esteban et al., 2015
2602	4.09	Esteban et al., 2015
2721	4.37	Esteban et al., 2015
3098	4.64	Esteban et al., 2015
3118	4.93	Esteban et al., 2015
3321	5.39	Esteban et al., 2015
4311	4.5	Esteban et al., 2015
3445	3.72	Esteban et al., 2015
3756	3.73	Esteban et al., 2015

3417	4.2	Esteban et al., 2015
3686	4.14	Esteban et al., 2015
4358	4.33	Esteban et al., 2015
3795	4.25	Esteban et al., 2015
3400	5.29	Esteban et al., 2015
3553	5.77	Esteban et al., 2015
3207	5.12	Esteban et al., 2015
3702	4.63	Esteban et al., 2015
3360	5.54	Esteban et al., 2015
3559	5.53	Esteban et al., 2015
3714	5.2	Esteban et al., 2015
4391	4.28	Esteban et al., 2015
3792	5.08	Esteban et al., 2015
3174	4.59	Esteban et al., 2015
3706	5.16	Esteban et al., 2015
3727	5.44	Esteban et al., 2015
4026	4.83	Esteban et al., 2015
4048	5.15	Esteban et al., 2015
3696	5.5	Esteban et al., 2015
3588	5.57	Esteban et al., 2015
4614	4.89	Esteban et al., 2015
4587	6.04	Esteban et al., 2015
4228	5.49	Esteban et al., 2015
4148	5.77	Esteban et al., 2015
3743	5.79	Esteban et al., 2015
3644	5.11	Esteban et al., 2015
3899	5.76	Esteban et al., 2015
3904	4.55	Esteban et al., 2015
3828	4.73	Esteban et al., 2015

3957	5.17	Esteban et al., 2015
4053	4.77	Esteban et al., 2015
3876	5.24	Esteban et al., 2015
4111	5.53	Esteban et al., 2015
4040	4.77	Esteban et al., 2015
4086	4.79	Esteban et al., 2015
4073	4.72	Esteban et al., 2015
4921	4.42	Esteban et al., 2015
4078	4.75	Esteban et al., 2015
4472	4.9	Esteban et al., 2015
4672	5.84	Esteban et al., 2015
4024	4.61	Esteban et al., 2015
4787	3.93	Esteban et al., 2015
3804	5.17	Esteban et al., 2015
3879	5.02	Esteban et al., 2015
4432	5.4	Esteban et al., 2015
2619	4.01	Esteban et al., 2015
2497	4.21	Esteban et al., 2015
2410	4.1	Esteban et al., 2015
2631	4.27	Esteban et al., 2015
3331	3.71	Esteban et al., 2015
3116	3.48	Esteban et al., 2015
2920	4.72	Esteban et al., 2015
2917	5.17	Esteban et al., 2015
2847	4.27	Esteban et al., 2015
3076	4.54	Esteban et al., 2015
2996	4.46	Esteban et al., 2015
3135	4.99	Esteban et al., 2015
3242	5.15	Esteban et al., 2015

2916	4.95	Esteban et al., 2015
2577	4.3	Esteban et al., 2015
3435	4.79	Esteban et al., 2015
3170	4.7	Esteban et al., 2015
5151	3.85	Esteban et al., 2015
3543	5.17	Esteban et al., 2015
3760	4.95	Esteban et al., 2015
4553	3.59	Esteban et al., 2015
3530	4.96	Esteban et al., 2015
4925	4.36	Esteban et al., 2015
3574	4.78	Esteban et al., 2015
3402	4.16	Esteban et al., 2015
3430	3.99	Esteban et al., 2015
4160	4.67	Esteban et al., 2015
4460	5.19	Esteban et al., 2015
3581	5.27	Esteban et al., 2015
4278	5.48	Esteban et al., 2015
4288	5.33	Esteban et al., 2015
3548	2.08	Esteban et al., 2015
5443	3.9	Esteban et al., 2015
3594	3.14	Esteban et al., 2015
3909	2.88	Esteban et al., 2015
4040	3.39	Esteban et al., 2015
3898	2.95	Esteban et al., 2015
5556	4.1	Esteban et al., 2015
4519	3.9	Esteban et al., 2015
4500	2.9	Esteban et al., 2015
3636	2.58	Esteban et al., 2015
4775	3.59	Esteban et al., 2015

4848	4.36	Esteban et al., 2015
3826	2.82	Esteban et al., 2015
4026	3.19	Esteban et al., 2015
3810	2.87	Esteban et al., 2015
4118	2.47	Esteban et al., 2015
3563	2.54	Esteban et al., 2015
3476	2.7	Esteban et al., 2015
4632	4.49	Esteban et al., 2015
4607	4.13	Esteban et al., 2015
5424	4.85	Esteban et al., 2015
4706	3.59	Esteban et al., 2015
4196	3.05	Esteban et al., 2015
4500	4.11	Esteban et al., 2015
5000	5.04	Esteban et al., 2015
4762	3.79	Esteban et al., 2015
4545	4.11	Esteban et al., 2015
4862	4.23	Esteban et al., 2015
4080	3.23	Esteban et al., 2015
4000	3.67	Esteban et al., 2015
3933	3.58	Esteban et al., 2015
3354	2.44	Esteban et al., 2015
3619	2.94	Esteban et al., 2015
4180	3.31	Esteban et al., 2015
4276	3.76	Esteban et al., 2015
4126	3.47	Esteban et al., 2015
3583	2.63	Esteban et al., 2015
4111	2.75	Esteban et al., 2015
3846	3.3	Esteban et al., 2015
4095	3.13	Esteban et al., 2015

4000	3.73	Esteban et al., 2015
3625	2.96	Esteban et al., 2015
5417	2.72	Esteban et al., 2015
3714	2.6	Esteban et al., 2015
3871	3.02	Esteban et al., 2015
3486	2.97	Esteban et al., 2015
3898	2.99	Esteban et al., 2015
3407	2.62	Esteban et al., 2015
3851	2.66	Esteban et al., 2015
3684	2.59	Esteban et al., 2015
3439	2.71	Esteban et al., 2015
4451	3.43	Esteban et al., 2015
4393	2.97	Esteban et al., 2015
3846	2.78	Esteban et al., 2015
3906	2.54	Esteban et al., 2015
4600	2.91	Esteban et al., 2015
3721	2.56	Esteban et al., 2015
3700	2.2	Esteban et al., 2015
4380	3.28	Esteban et al., 2015
4353	3.02	Esteban et al., 2015
3846	2.69	Esteban et al., 2015
4000	2.77	Esteban et al., 2015
4067	2.35	Esteban et al., 2015
3708	2.54	Esteban et al., 2015
5385	4.07	Esteban et al., 2015
3714	2.5	Esteban et al., 2015
2930	3.59	Mielke et al., 2017
3280	3.65	Mielke et al., 2017
3130	3.56	Mielke et al., 2017

3160	3.77	Mielke et al., 2017
3370	3.62	Mielke et al., 2017
3300	3.09	Mielke et al., 2017
3320	3.24	Mielke et al., 2017
3360	3.35	Mielke et al., 2017
3380	3.2	Mielke et al., 2017
3530	3.18	Mielke et al., 2017
3820	3.46	Mielke et al., 2017
3680	3.35	Mielke et al., 2017
3780	3.21	Mielke et al., 2017
3600	3.37	Mielke et al., 2017
5740	3.23	Mielke et al., 2017
5740	3.32	Mielke et al., 2017
5460	3.36	Mielke et al., 2017
5630	3.36	Mielke et al., 2017
5960	3.47	Mielke et al., 2017
5710	3.49	Mielke et al., 2017
5720	3.46	Mielke et al., 2017
4980	3.5	Mielke et al., 2017
6310	3.61	Mielke et al., 2017
4820	3.35	Mielke et al., 2017
5380	3.82	Mielke et al., 2017
5770	3.69	Mielke et al., 2017
5930	3.58	Mielke et al., 2017
6170	3.78	Mielke et al., 2017
5640	3.79	Mielke et al., 2017
6140	3.67	Mielke et al., 2017
4070	3.52	Mielke et al., 2017
3990	3.55	Mielke et al., 2017

4170	3.59	Mielke et al., 2017
4310	3.66	Mielke et al., 2017
4260	3.66	Mielke et al., 2017
4070	3.64	Mielke et al., 2017
4040	3.57	Mielke et al., 2017
4230	3.66	Mielke et al., 2017
4060	3.44	Mielke et al., 2017
4200	3.48	Mielke et al., 2017
3910	3.76	Mielke et al., 2017
4020	3.7	Mielke et al., 2017
3930	3.61	Mielke et al., 2017
4320	3.71	Mielke et al., 2017
3950	3.78	Mielke et al., 2017
4330	3.69	Mielke et al., 2017
3720	3.59	Mielke et al., 2017
4420	3.81	Mielke et al., 2017
4760	3.82	Mielke et al., 2017
2820	3.43	Mielke et al., 2017
2870	3.38	Mielke et al., 2017
2850	3.58	Mielke et al., 2017
3110	3.71	Mielke et al., 2017
3390	3.75	Mielke et al., 2017
3040	3.48	Mielke et al., 2017
3070	3.49	Mielke et al., 2017
3600	3.66	Mielke et al., 2017
4130	3.98	Mielke et al., 2017
4010	3.62	Mielke et al., 2017
4040	4.12	Mielke et al., 2017
3980	3.76	Mielke et al., 2017

4270	4	Mielke et al., 2017
2880	3.51	Mielke et al., 2017
3100	3.74	Mielke et al., 2017
3370	3.69	Mielke et al., 2017
3240	3.78	Mielke et al., 2017
3030	3.74	Mielke et al., 2017
3080	3.73	Mielke et al., 2017
3180	3.59	Mielke et al., 2017
3420	3.83	Mielke et al., 2017
3210	3.78	Mielke et al., 2017
3490	3.71	Mielke et al., 2017
3390	3.85	Mielke et al., 2017
3480	3.89	Mielke et al., 2017
3820	3.9	Mielke et al., 2017
3690	3.98	Mielke et al., 2017
3980	4.07	Mielke et al., 2017
3930	4.06	Mielke et al., 2017
3780	4.03	Mielke et al., 2017
4520	3.75	Mielke et al., 2017
4320	3.93	Mielke et al., 2017
4180	3.77	Mielke et al., 2017
5100	3.8	Mielke et al., 2017
3780	3.99	Mielke et al., 2017
4470	3.8	Mielke et al., 2017
4540	4	Mielke et al., 2017
4230	3.88	Mielke et al., 2017
3940	4.32	Mielke et al., 2017
3590	4.41	Mielke et al., 2017
3740	4.03	Mielke et al., 2017

3360	4.34	Mielke et al., 2017
4430	3.75	Mielke et al., 2017
3800	4.25	Mielke et al., 2017
3930	4.54	Mielke et al., 2017
3650	4.27	Mielke et al., 2017
4030	4.21	Mielke et al., 2017
3940	4.39	Mielke et al., 2017
5280	3.81	Mielke et al., 2017
4330	4.47	Mielke et al., 2017
4620	3.82	Mielke et al., 2017
4560	3.73	Mielke et al., 2017
4150	4.36	Mielke et al., 2017
4400	4.59	Mielke et al., 2017
4070	4.51	Mielke et al., 2017
4640	3.72	Mielke et al., 2017
4310	3.63	Mielke et al., 2017
4610	4.37	Mielke et al., 2017
5210	3.8	Mielke et al., 2017
3694.077	5.450539	Zamora et al., 1993
4394.21	6.172434	Zamora et al., 1993
5255.347	6.871188	Zamora et al., 1993
4800	3.02	Pimienta et al., 2018
5640	3.58	Pimienta et al., 2018
4970	3.16	Pimienta et al., 2018
5550	3.46	Pimienta et al., 2018
4390	2.98	Pimienta et al., 2018
4500	2.79	Pimienta et al., 2018
4190	2.84	Pimienta et al., 2018
4490	2.84	Pimienta et al., 2018

4110	3	Pimienta et al., 2018
4200	3.43	Pimienta et al., 2018
4210	3.01	Pimienta et al., 2018
4270	2.95	Pimienta et al., 2018
2650	2.76	Pimienta et al., 2018
2770	2.89	Pimienta et al., 2018
1580	2.84	Pimienta et al., 2018
1460	2.73	Pimienta et al., 2018
3260	1.82	Pimienta et al., 2018
2220	2.19	Pimienta et al., 2018
3510	2.18	Pimienta et al., 2018
4410	1.22	Pimienta et al., 2018
5510	2.24	Pimienta et al., 2018
3020	1.71	Pimienta et al., 2018
3290	1.85	Pimienta et al., 2018
4740	2.41	Pimienta et al., 2018
3180	2.31	Pimienta et al., 2018
4575.783	4.149969	Duffaut et al., 2018
4650.296	2.185838	Duffaut et al., 2018
2882.303	1.587199	Duffaut et al., 2018
2563.929	1.320037	Duffaut et al., 2018
2753.599	1.6812	Duffaut et al., 2018
3969.517	2.279839	Duffaut et al., 2018
4633.361	2.927953	Duffaut et al., 2018
3651.143	2.56679	Duffaut et al., 2018
3414.056	2.77953	Duffaut et al., 2018
3654.53	3.299011	Duffaut et al., 2018
4403.048	3.036797	Duffaut et al., 2018
3498.73	1.517934	Duffaut et al., 2018

2814.564	1.339827	Duffaut et al., 2018
2638.442	1.156772	Duffaut et al., 2018
2516.512	0.939085	Duffaut et al., 2018
2486.029	1.310142	Duffaut et al., 2018
2530.059	1.409091	Duffaut et al., 2018
3041.49	1.557514	Duffaut et al., 2018
3146.486	1.364564	Duffaut et al., 2018
3661.304	1.987941	Duffaut et al., 2018
3651.143	1.562461	Duffaut et al., 2018
3698.561	1.097403	Duffaut et al., 2018
4494.496	1.458565	Duffaut et al., 2018
3996.613	1.428881	Duffaut et al., 2018
2980.525	1.310142	Duffaut et al., 2018
2790.855	1.018244	Duffaut et al., 2018
3471.634	1.31509	Duffaut et al., 2018
6993.311	3.344961	Leadholm et al., 1985
4899.666	3.689833	Leadholm et al., 1985
4678.93	3.684607	Leadholm et al., 1985
5307.692	3.324059	Leadholm et al., 1985
5501.672	3.21694	Leadholm et al., 1985
5501.672	3.167299	Leadholm et al., 1985
5494.983	3.133334	Leadholm et al., 1985
5394.649	3.209102	Leadholm et al., 1985
5374.582	3.167299	Leadholm et al., 1985
5294.315	3.224778	Leadholm et al., 1985
5280.937	3.193426	Leadholm et al., 1985
5307.692	3.094145	Leadholm et al., 1985
5301.003	3.133334	Leadholm et al., 1985
5314.381	3.049729	Leadholm et al., 1985

5240.803	3.052342	Leadholm et al., 1985
5066.89	3.167299	Leadholm et al., 1985
5013.378	3.164686	Leadholm et al., 1985
5013.378	3.143785	Leadholm et al., 1985
5060.201	3.141173	Leadholm et al., 1985
5086.957	3.010539	Leadholm et al., 1985
4879.599	3.086307	Leadholm et al., 1985
3782.609	3.175137	Leadholm et al., 1985
3782.609	2.960899	Leadholm et al., 1985
4284.281	2.924321	Leadholm et al., 1985
4886.288	2.783237	Leadholm et al., 1985
4973.244	2.673505	Leadholm et al., 1985
4625.418	2.574224	Leadholm et al., 1985
4357.859	2.582062	Leadholm et al., 1985
4284.281	2.670892	Leadholm et al., 1985
3983.278	2.715308	Leadholm et al., 1985
3795.987	2.681343	Leadholm et al., 1985
3675.585	2.62909	Leadholm et al., 1985
3274.248	2.083042	Leadholm et al., 1985
3187.291	1.834839	Leadholm et al., 1985
3361.204	1.73817	Leadholm et al., 1985
3254.181	1.584023	Leadholm et al., 1985
3073.579	1.748621	Leadholm et al., 1985
2765.886	1.667628	Leadholm et al., 1985
2284.281	1.910606	Leadholm et al., 1985
2297.659	1.746008	Leadholm et al., 1985
2183.947	1.701593	Leadholm et al., 1985
2277.592	1.667628	Leadholm et al., 1985
2277.592	1.500418	Leadholm et al., 1985

2163.88	1.479516	Leadholm et al., 1985
1822.742	1.495192	Leadholm et al., 1985

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Appendix 3 – Co-authored paper

Shallow gas and gas hydrate occurrences on the northwest Greenland shelf margin

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Abstract

Industrial 3D seismic data are used to investigate the contemporary hydrocarbon distribution and historical fluid migration in Melville Bay offshore northwest Greenland. Gas-related amplitude anomalies and an extensive bottom simulating reflector (BSR) were mapped within the uppermost 1-2 km of stratigraphy to define the first inventory of shallow gas and gas hydrate along this part of the Greenland margin. The shallow gas anomalies vary in seismic character and have been subdivided into four categories that represent (I) isolated shallow gas, (II) free gas trapped at the base of the gas hydrate stability zone (GHSZ), (III) gas charged glacial clinoforms and (IV) a giant mass transport deposit gas reservoir. Gas hydrate deposits have been identified across an area of 537 km² via the identification of a discontinuous BSR that marks the base of the GHSZ. The BSR has been used to estimate a geothermal gradient of 49 °C/km across the GHSZ and a heat flow of 70-90 mW/m², providing the first publically available heat flow estimates offshore western Greenland. The contemporary hydrocarbon distribution and historical fluid migration is influenced by the underlying paleo-rift topography and multiple shelf edge glaciations since ~2.7 Ma. Continued uplift of the Melville Bay Ridge, as well as glacial-sediment redistribution and basinward margin tilting from isostatic compensation, have led to a concentration of hydrocarbons within the Cenozoic stratigraphy above the ridge. Furthermore, repeated variations in subsurface conditions during glacial-interglacial cycles likely promoted fluid remigration, and possibly contributed to reservoir leakage and increased fluid migration through faults. The top of the gas hydrate occurrence at 650 m water depth is well below the hydrate-free gas phase boundary (~350 m) for the present bottom-water temperature of 1.5 °C, suggesting this hydrate province mainly adjusted to glacial-interglacial changes by expansion and dissociation at its base and is relatively inert to current levels of global warming. This glacial-related dissociation may have significantly contributed to the numerous free gas accumulations observed below the GHSZ at present day.

Key Words (max 6)

Shallow gas, gas hydrate, seismic anomalies, fluid migration, bottom simulating reflector, glaciation

1. Introduction

Gas-rich sediments have been documented on most continental shelf margins worldwide (Fleischer et al., 2001), with these accumulations predominantly representing thermogenically or biogenically generated shallow gas or gas hydrate deposits (Floodgate and Judd, 1992; Kvenvolden, 1993; Minshull et al., 2020; Schoell, 1988; Stopler et al., 2014). These deposits have attracted considerable interest over the last few decades as they: (1) represent potential drilling hazards (McConnell et al., 2012; Merey, 2016; Prince, 1990); (2) can impact the stability of seafloor sediments (Brown et al., 2006; Yang et al., 2018); (3) have been considered as a future lower-carbon energy source (Collett et al., 2009; Demirbas, 2010; McGlade and Ekins, 2015); (4) can be used to indirectly estimate shallow geothermal gradient and heat flow through identified bottom simulating reflectors (BSRs) (Dickens and Quinby-Hunt, 1994; Grevemeyer and Villinger, 2001); and (5), since methane is a powerful greenhouse gas, hydrate dissociation may pose a positive feedback mechanism for global climate warming, especially when found in relatively shallow water depths (Karisiddaiah and Veerayya, 1994; Krey et al., 2009; Ruppel and Kessler, 2017; Zhao et al., 2017).

For these reasons, it is important to document and understand the distribution of shallow gas and gas hydrates, especially within high latitude environments sensitive to environmental change (Portnov et al., 2016). Understanding high latitude hydrocarbon systems can be difficult, however, as glaciations during the Pliocene-Pleistocene may have significantly influenced fluid migration (Goffey et al., 2016; Medvedev et al., 2019). The redistribution of sediment across glaciated margins, along with repeated ice loading and unloading on the shelf through glacial-interglacial cycles, can cause substantial structural changes, isostatic compensation, and significant variations in subsurface conditions (Fjeldskaar and Amantov, 2018; Zieba and Grover, 2016). These changes often promote the remigration of hydrocarbons, through processes such as fault reactivation, trap spill and seal breach, potentially leading to expulsion at the seabed into the water column (Goffey et al., 2016; Kjemperud and Fjeldskaar, 1992; Ostanin et al., 2017). Gas hydrate stability is also affected by variations in subsurface temperature and pressure (Kvenvolden, 1993), such as those related to glacial (un)loading, and can possibly lead to dissociation of hydrate at the seabed (Andreassen et al., 2017; Grassmann et al., 2010). Attempting to understand this cryosphere-methane interaction may reveal the sensitivity of gas hydrate deposits to environmental change; providing critical insight into how these deposits may respond to future oceanic warming (Biastoch et al., 2011; Krey et al., 2009; Ruppel and Kessler, 2017).

The Melville Bay continental margin, offshore northwest Greenland, has experienced multiple episodes of ice sheet advance and retreat across the shelf since ~2.7 Ma, with sediment redistribution contributing to ~100 km of shelf edge progradation (Figs. 1 and 2) (Knutz et al., 2019; Newton et al., 2020; 2017). The region is thought to contain hydrocarbon systems (Bojesen-Koefoed, 2011; Gregersen et al., 2013; Whittaker et al., 1997) that were likely impacted by these glaciations. Here, extensive 3D seismic reflection data acquired for petroleum exploration are used to document the structure, stratigraphy and hydrocarbon occurrence across the glaciated margin of Melville Bay. The data coverage and mapping provides the most widespread and high-resolution imaging of the subsurface and hydrocarbon anomalies along the west coast of Greenland, as well as the most northerly documentation of gas hydrates in Baffin Bay (Minshull et al., 2020; Nielsen et al., 2014). The primary objectives were to address: (1) Have hydrocarbons accumulated within shallow, post-rift sediments on the Melville Bay shelf; (2) What does the seismic character and distribution of observed

hydrocarbon occurrences tell us about migration history; and (3) How have these accumulations been affected by recent glaciations? In addition to answering these questions, the analysis contributes to the wider understanding of Arctic gas hydrates, the West Greenland subsurface thermal regime and shallow subsurface drilling hazards for the upcoming IODP Leg (909) (Knutz et al., 2018).

2.Regional setting

Baffin Bay represents a large marginal sea between Greenland and Canada that formed during the early phase (Paleocene-Eocene) of North Atlantic opening (Gregersen et al., 2013; Oakey and Chalmers, 2012). Melville Bay is located in northeast Baffin Bay and overlies large areas of the northwest Greenland rifted continental margin (Fig. 1). The shelf area of Melville Bay is characterised by deep sedimentary basins, with thicknesses >10 km, separated by extensive elongate ridges (Gregersen et al., 2019; Whittaker et al., 1997), with this complex paleo-rift topography overlain by a thick (1-3 km) Cenozoic post-rift succession (Fig. 2) (Gregersen et al., 2013; Knutz et al., 2012; 2015; 2019).

Figure 1. Location Map. Bathymetric map from Newton et al. (2017) of the Melville Bay region offshore northwest Greenland (see insert map), displaying the location of seismic data as well as the influence of repeated glaciations on margin architecture. Black labels indicate the location of paleo-rift topography and deep rift basins across the shelf. SKB = South Kivioq Basin. MBG = Melville Bay Graben.

Stratigraphic Framework

The rift and post-rift succession of the northwest Greenland continental margin has been mapped extensively and subdivided into seven seismic mega-units (mu) (A-G) bounded by regional horizons with up-dip unconformable expressions (Gregersen et al., 2013; 2016; Knutz et al., 2015) (Fig. 2). This regional seismic-stratigraphic framework for West Greenland has been adopted as a basis for a detailed 3D seismic analysis of the uppermost (1-2 km) stratigraphic packages.

Proterozoic aged basement (mu-H) underlies Early Cretaceous-early Paleocene syn-rift sedimentary rocks that make up mu-G and -F (Cox et al., 2020a; Gregersen et al., 2019; 2013). These sediments likely consist of marine mudstones intercalated with sandy deposits, as well as possible organic shales (source rocks) within mu-F, which may have been deposited during a period of rift quiescence during the Cenomanian-Turonian (Bojesen-Koefoed et al., 1999; Cox et al., 2020a; Nohr-Hansen et al., 2018; Planke et al., 2009).

Figure 2. Regional stratigraphy. (A) Uninterpreted regional 2D seismic reflection line in two-way-time, displaying the stratigraphy across the Melville Bay continental shelf. (B) An interpreted version of (A) defining the character of the regional stratigraphy including deep rift basins, the prominent Melville Bay Ridge and the thick package of glacigenic sediments. Nine seismic mega-units (mu-H to -A) as well as top unit horizons (horizon hx to b1) are defined, based on Gregersen (2013; 2017) and Knutz et al. (2015). The occurrence of potential seismic fluid anomalies, faults and possible organic rich Cretaceous strata are also shown. The location of the seismic line is shown on Figure 1.

The oldest section of the post-rift succession is represented by mu-E and consists mainly of hemipelagic marine mudstones intercalated with submarine fan deposits (Knutz et al., submitted). The mu-E succession was deposited during the seafloor spreading phase of Baffin Bay (syn-drift), followed by mu-D, of likely late Eocene to early-middle Miocene age. The lower part of mu-D consists of asymmetric wedges of submarine fans that possibly formed as a result of inversion as Greenland and North America converged and spreading in Baffin Bay ceased (Knutz et al., 2012; submitted). The upper part of mu-D displays a hemipelagic infill character, presumably with a high clay content facilitating the development of polygonal fault networks

(Goulty and Swarbrick, 2005). Mu-D thins significantly above the crest of the Melville Bay Ridge (MBR) and is top bounded by a regional unconformity (horizon d1) (Fig. 2) (Cox et al., 2020a; Gregersen et al., 2019; Knutz et al., 2012). This thinning package represents the seal for a gas-charged mass transport deposit covering 420 km² of the MBR crest (within mu-D2) (Fig. 2). The reservoir displays seismic characteristics interpreted as direct hydrocarbon indicators and was likely deposited as a shallow marine spit complex along the ridge axis during the Eocene (Cox et al., 2020a). Reservoir deformation and transport occurred along a muddy décollement layer that represents horizon e1; an important unconformity that marks the top of the MBR structure and the transition from syn- to post-rift sedimentation (Gregersen et al., 2019).

On the inner shelf, the uppermost post-rift succession consists of extensive, thick marine sediment packages that were deposited during the late Miocene and Pliocene (mu-C and mu-B) (Knutz et al., 2015) (Fig. 2), and have been heavily truncated by glacial erosion. Mu-C, which buried the MBR, is interpreted as a deep shelf drift accumulation influenced by northward flowing ocean currents (Knutz et al., 2015; 2019). Mu-B is considered mainly Pliocene in age and displays mounded and wavy depositional features that preferentially infilled erosional scarps where large parts of mu-C had been removed (Fig. 2). Basinward, the contourite accumulations and their correlative downslope mass transport deposits are buried progressively deeper by the thick glaciogenic packages of mu-A corresponding to the Melville Bay Trough Mouth Fan (Knutz et al., 2019) (Fig. 2). The progradational succession of mu-A has been subdivided into 11 units reflecting deposition by migrating ice-streams since the late Pliocene (Knutz et al., 2019; Newton et al., 2020).

Structural Framework

The paleo-rift topography consists of northwest-southeast trending elongate ridges formed during Early Cretaceous to early Paleogene syn-rift phases (Figs. 2 and 3) (Gregersen et al., 2013; 2016; Larsen et al., 2009; Whittaker et al., 1997). The Kivioq Ridge, located beneath the present outer shelf margin, and the MBR, separate the main depocentres of the Melville Bay Graben and South Kivioq Basin (Figs. 2 and 3) (Cox et al., 2020a; Gregersen et al., 2013; 2016; Knutz et al., 2015). The ~200 km long MBR has continued as a positive relief feature into the Neogene, long after rifting ceased in the late Eocene/early Oligocene (Oakey and Chalmers, 2012; Welford et al., 2018). Consequently, the flanks of the MBR are onlapped and in parts draped by both syn- and post-rift sedimentary successions (Fig. 2) with potential implications for regional fluid migration.

Figure 3. Structural framework across the northern section of the study area. A two-way-time structure map of horizon e1 has been used to define the location of the Melville Bay Ridge. The location of deep tectonic faults (black) (including the western ridge fault) and post-rift faults (white) are shown, with the faults observed to strike parallel to ridge strike. Two windows (to scale) displaying seismic variance time slices from depths of 1600 ms TWT (Pitu) and 2230 ms TWT (Anu), display a network of thin, curvilinear high amplitude features that represent the polygonal fault network that exists within mu-D and -C, with the location of these faults across the area shown by the diagonal hatch. The location of Figures 4, 9A, 9C, 15 and a section of 2 are shown.

The MBR and Kivioq Ridge are characterised by numerous internal and ridge bounding deep tectonic normal faults generally oriented parallel to the ridge strike (Figs. 2 and 3) (Gregersen et al., 2019). The MBR formed as an elongate tilted fault block, with large offsets and disconnected syn-rift stratigraphy on its western flank adjoining the ‘western ridge fault’ (Figs. 2 and 3). This is contrasted by a steeply dipping stratigraphy to the east that continues into the Melville Bay Graben (Fig. 2 and 3).

The deep pre- and syn-rift tectonic faults extend vertically to the horizon e1 unconformity marking the MBR apex (Fig. 2) (Gregersen et al., 2019). This horizon acts as a boundary

between the deeper faults and a dense fault network within the post-rift stratigraphy (above horizon d2; Fig. 2). As well as tectonic faults, the 3D seismic mapping revealed that a large proportion of post-rift faults, especially within the grabens, exist as closely spaced, short offset faults that likely represent an intra-formational polygonal fault network formed by compactional processes, e.g. shale dewatering and diagenesis, (Fig. 2 and 3) (Cartwright and Dewhurst, 1998; Cox et al., 2020a). A neo-tectonic influence on the ridge complex is suggested by the observation that faults intersecting mu-D and -C over the ridge flanks often extend from deeper structural features (Fig. 2).

3. Materials and methods

3.1 Seismic and Velocity Data

The main database for this study consists of two 3D seismic reflection datasets and one regional 2D seismic reflection grid that covers much of the continental shelf in Melville Bay (Fig. 1). The first 3D seismic reflection survey (Pitu) was acquired by Cairn Energy in 2011 and covers an area of 1,672 km². It is provided in two-way time (TWT) down to 6.5 seconds and was acquired using 93 3D acquisition lines with 25 x 12.5 m bin spacing and a line separation of 1 km. A 25 m shot point interval (flip flop) was used with a 50 m source separation creating a common-mid-point fold of 70. Ten 7050 m long streamers were used, each with 564 channels and towed at a depth of 20 m. The dominant frequency varies with depth but is 28 Hz at approximately 1500 ms TWT, producing a dominant wavelength of 71 m (using an average velocity of 2.0 km/s) and a vertical resolution of 18 m. The reprocessing of this survey in 2013 provided a sub-set high resolution 3D seismic survey in TWT (Pitu HR survey) that covers an area of 1,135.5 km² down to 5 seconds TWT. The resolution of the data has been improved to a spatial resolution of 12.5 m (inline) x 6.25 m (crossline) and a vertical resolution of 11 m at the same stratigraphic interval (~1500 ms TWT) due to a dominant frequency of 45 Hz and a dominant wavelength of 44 m.

The processing of the Pitu survey involved noise attenuation and filtering, 3D deconvolution, Pre-Stack Depth Migration (PSDM), post-migration velocity analysis and a parabolic radon de-multiple process. An understanding of the velocity field was gained during the PSDM of the full survey, which involved an iterative velocity investigation including multi-layer tomography to minimise residual move-out, stack scanning to help flatten irregular unconformities and finally Kirchhoff pre-stack Tilted Transverse Isotropy (TTI) depth migration, creating a depth domain volume which was subsequently converted into the time domain. This process produced an interval velocity cube based solely on seismic velocities (Fig. 4) as well as a depth domain seismic volume down to 10 km. An assessment of the accuracy of both the depth conversion and interval velocity cube is not possible as no calibration data (such as boreholes) exist in the area for comparison. However, interval velocity variations show a good correlation to both regional 2D stacking velocities and the location of regional unconformities (where rapid increase in velocity may be expected), such as at the top of the MBR (horizon e1) (Fig. 4).

Figure 4. Seismic cross section from the Pitu HR survey demonstrating the relationship between seismic stratigraphy, interval velocity and potential gas hydrate deposits. The seismic amplitudes are overlain by a semi-transparent cross section displaying the corresponding interval velocity. Key seismic horizons and a bottom simulating reflector (BSR), marking the base of the gas hydrate stability zone (GHSZ), are indicated. 1D interval velocity profiles display the variation of velocity through the GHSZ and the adjacent stratigraphy. The cross section location is shown on Figure 3.

The second 3D seismic reflection survey (Anu) was acquired by Shell in 2013 over an area of 8700 km² (Fig. 1). It is provided in TWT down to 7.5 seconds and was acquired using 118 sail lines with a 50 m (cross-line) x 6.25 m (inline) bin spacing and a line separation of 600 m. The acquisition used a dual vessel set-up with six, 7050 m long streamers (each with 564 channels) that were separated by 200 m and towed at a depth of 10 (front end) to 15 m (tail end). Two sources were separated by 100 m at a depth of 8 m and were fired using a shot point interval (flip flop) of 25 m, producing a nominal fold coverage of 70. The processing workflow included noise and acquisition footprint attenuation processes, multiple removal using both 3D surface related multiple reflection (SRME) and 2D model-based water-layer de-multiple (MWD) modelling, a 1 km migration velocity analysis and a final isotropic Kirchhoff pre-stack time migration (PSTM). This produced a volume with a dominant frequency of 30 Hz at approximately 1500 ms TWT, a dominant wavelength of 67 m (using an average velocity of 2.0 km/s) and a vertical resolution of 17 m.

The 15 lines of 2D seismic reflection data used were acquired by TGS between 2007 and 2009 and form part of the Baffin Bay 2D (BBRE11) regional dataset (Fig. 1). The lines used here cover 5,038 km and were acquired using a single 6000 m streamer with 480 channels, 12.5 m intervals and a sampling rate of 2 ms, as well as a 2000 psi source with a 25 m interval at a gun depth of 8 m, yielding a 120-fold stack. The survey was reprocessed in 2011 to boost low frequencies and enhance resolution, specifically targeting multiple and bubble pulse attenuation. The processing sequence involved a 2 km Kirchhoff pre-stack curved ray time migration and velocity analysis within this process produced stacking velocity data for each 2D line.

All data used were provided in SEG normal polarity with a downward increase in acoustic impedance (such as at the seabed) represented by a red positive peak and a downward

decrease in acoustic impedance represented by a blue negative trough (Fig. 5). No well data were available within the area of interest.

3.2 Interpretation Methods

The regional structural and stratigraphic framework (Gregersen et al., 2013; 2016; Knutz et al., 2015) was propagated through the 3D seismic data using Schlumberger's Petrel software and standard 3D seismic interpretation techniques (Cox et al., 2020b; Posamentier, 2004; Posamentier et al., 2007). This study focused on the mapping of features such as seismic discontinuities and amplitude anomalies that could be linked with fluid migration and hydrocarbon accumulations (Hilterman, 2001). Analysis of such features found that likely gas-related anomalies often displayed seismic amplitudes larger than -10,000 (Fig. 5), although dimmer anomalies may also comprise shallow gas accumulations associated with saturations of less than 10%, poorer reservoir quality or thin-bed effects (Hilterman, 2001), and this was considered when filtering results. Using this understanding of anomaly amplitude, automated anomaly detection and filtering was applied to the 3D data via the method described in Cox et al. (in press) (Fig. 5). The individual scrutiny of each anomaly within the filtered results was then conducted to determine whether that anomaly was in fact fluid-related or created by another feature.

Figure 5. A seismic cross section (A) illustrating the method of using proportional minimum amplitude extraction windows to identify shallow gas anomalies. Examples of isolated anomalies are shown (category I). The polarity of seismic data used in this study is shown with an increase in acoustic impedance at the seabed representing a positive amplitude brown-red-yellow peak. The location of the line is shown on Figure 7. (B) Histogram of the amplitude distribution from an extracted minimum amplitude window, demonstrating the filtering process for isolating the seismic signal most likely representing shallow gas occurrences.

Non-fluid-related bright 'soft' amplitude anomalies may represent features such as high porosity, low density and low velocity (i.e. low acoustic impedance) stratigraphic layers such as diatomaceous ooze or coal beds, organic-rich claystones, and data acquisition footprint (stronger near the seabed) (Cox et al., in press). Distinguishing between fluid-related and lithology-related anomalies, for example those created by low density oozes which may create similar amplitudes, is sometimes difficult, but can usually be distinguished based on context as lithological variations are more often stratigraphically restricted and more widespread, e.g.

Batchelor et al. (2017). This evaluation is therefore somewhat subjective, increasing uncertainty, and this should be considered in the final result. Additionally, high saturation gas anomalies have likely been detected efficiently through this process, but the number of fluid-related anomalies may be underestimated, as very thin (few metres) or very low saturation gas pockets (<<5%), causing only low amplitude seismic anomalies, may have been omitted.

3.3 Geothermal Gradient and Heat Flow Calculations

Near surface geothermal gradient and heat flow were estimated across part of the Pitu 3D seismic survey area using an identified BSR that is thought to represent the base of the gas hydrate stability zone (GHSZ) (Dickens and Quinby-Hunt, 1994; Grevenmeyer and Villinger, 2001). Gas hydrate stability is influenced by fluid composition, pressure and temperature conditions (Kvenvolden, 1993), and the estimation requires key parameters including temperature at the seabed and BSR, as well as the thermal conductivity of the shallow gas hydrate hosting sediments (Grevenmeyer and Villinger, 2001; Minshull and Keddle, 2010). These parameters are often provided by seabed and downhole temperature probes and logging data. However, no such data exist in northeast Baffin Bay, so these essential parameters have to be either extracted from interpolated global databases or from published gas hydrate stability models and empirical relationships using the constraints provided by the seismic data (TWT and depth of seabed and BSR, interval velocity of the GHSZ).

Estimating parameters in such ways creates uncertainty - e.g. estimating heat flow without direct temperature data is thought to cause an error of 20% or above, whilst the estimation of thermal conductivity through empirical relationships instead of seabed measurements, can cause errors of 5-30% (Grevenmeyer and Villinger, 2001; Minshull, 2011). Other uncertainties arise from seismic interpretation errors, velocity model creation and depth conversion and uncertainty of the true phase boundary depth, due to an unknown composition of pore water and hydrate (other gases such as hydrogen sulphide or higher order hydrocarbons can affect the phase boundary) (Grevenmeyer and Villinger, 2001; Minshull, 2011; Minshull and Keddle, 2010). Error resulting from these uncertainties is often over 10%, with the compound uncertainty being potentially large (e.g. > 50% cf. Grevenmeyer and Villinger 2001), but in areas where no data exist, an estimate with recognised uncertainty is better than no information at all. The geothermal gradient and heat flow were estimated using the procedure described by several authors (Dickens and Quinby-Hunt, 1994; Grevenmeyer and Villinger, 2001; Yamano et al., 1982) and used within a number of similar studies (Calves et al., 2010; Minshull and Keddle, 2010; Serié et al., 2017; Shankar et al., 2010).

It was assumed that hydrate gas is pure methane and the pore water exhibits normal sea-water salinity – this is the most commonly observed scenario and thus a typical assumption when no borehole data are available (Dickens and Quinby-Hunt, 1994; Shankar et al., 2010). There is a chance of higher order hydrocarbons, with the hydrate forming gas potentially sourced from Cretaceous marine source rocks (Cox et al., 2020a; Nohr-Hansen et al., 2018), however, no ‘double-BSR’ is observed that may suggest the presence of three fluid phases (Andreassen et al., 2000; Geletti and Busetti, 2011). The first step was to interpret the seabed and the BSR on the Pitu depth domain seismic. The pressure (p) at the BSR was then calculated using Equation 1, which represents a standard hydrostatic pressure equation (Dickens and Quinby-Hunt, 1994). This used an estimated seawater density of 1034 kg/m³ for relatively deep, saline and cold ocean bottom waters on the Melville Bay shelf provided by Tang et al. (2004). The pressure equation assumes hydrostatic pressure at the BSR depth and therefore depth is measured from mean sea level.

Equation 1: BSR Pressure (p) = $(1034 * 9.81 * \text{BSR Depth}) / -1000000$

Units: Seawater density = 1034 kg/m³ Gravity = 9.81 m/s²
Megapascals (MPa) conversion = 1000000

The temperature at the BSR was estimated from the calculated pressure using Equation 2. This equation is based on an empirical relationship between pressure and dissociation temperature, defined by experimental data for various methane hydrate stability conditions, with a regression showing a Chi-squared of >0.99 (Dickens and Quinby-Hunt, 1994). Equation 2 represents this empirical relationship rearranged to find the dissociation temperature for any pressure between 2.5-10 MPa. The only variable in the equation is pressure, with the values 0.00379 and 0.000283 representing constants derived from the original empirical relationship.

Equation 2: BSR Temperature = $(1/((0.00379) - (0.000283 * \text{Log}(\text{BSR Pressure})))) - 273$

Units: BSR Pressure (p) = MPa °C conversion = -273

The temperature change across the GHSZ was then calculated by subtracting the seabed temperature which was estimated from the world ocean temperature database (Locarnini et al., 2013), showing an annual mean temperature of ~1.5 °C for ocean bottom waters at this depth (~650 m) across Melville Bay. The seabed elevation varies in depth by ~100 m across the BSR area and therefore, this temperature may vary slightly (less than 0.5 °C), translating to a BSR temperature error of < +/- 0.2 °C. The temperature difference across the GHSZ was then divided by the thickness (in metres) (Equation 3) to calculate the Geothermal Gradient (Dickens and Quinby-Hunt, 1994; Grevemeyer and Villinger, 2001).

Equation 3: Geothermal Gradient = $\frac{(\text{BSR Temperature} - \text{Seabed Temperature})}{(\text{BSR Depth} - \text{Seabed Depth})}$

Units: BSR/Seabed Temperature = °C BSR/Seabed Depth = m

Heat flow across the same zone was then derived from the estimated geothermal gradient. This requires an understanding of the thermal conductivity structure of the GHSZ. In the absence of borehole control, an empirical relationship between interval velocities and thermal conductivity (k) is used, that was derived from a number of experimental datasets (filtered to only include wet samples to represent subsurface fluid saturation) that include P-wave velocity, thermal conductivity and porosity measurements across a wide range of lithologies, e.g. Grevemeyer and Villinger (2001), Boulanouar et al. (2013) and Esteban et al. (2015). This relationship was used to estimate the thermal conductivity of the shallow sediments as a function of the seismically-defined interval velocities of the GHSZ (Equation 4). The empirical relationship is represented by 0.5071 in equation 4, which is the intercept of the regression equation through the selected experimental data points. Within equation 4, the interval velocities are multiplied by 0.001 to convert from m/s to km/s to ensure the thermal conductivity units match those of geothermal gradient and heat flow.

Equation 4: Thermal Conductivity (k) = $(\text{Interval Velocity} * 0.001) - 0.5071$

Units: k = W/m⁻¹/K⁻¹ Interval Velocity = m/s

The final step was to use the thermal conductivity and the geothermal gradient to calculate heat flow (Q) through the GHSZ using Fourier's Law (Equation 5). It should be noted, as acknowledged above, that the compound uncertainties may be as much as 50-60 % on the final heat flow estimates (Grevemeyer and Villinger, 2001).

Equation 5: Heat Flow (Q) = Geothermal Gradient * Thermal Conductivity (k)

Units: Q = mWm⁻² GTG = °C/m k = W/m⁻¹/K⁻¹

4.Results

4.1 Shallow Gas

Numerous, scattered seismic anomalies are observed within the Cenozoic sedimentary succession covering the rift basins of Melville Bay (Fig. 6 and 7) and potentially represent the presence of free gas or gas-rich pore fluids. The identified acoustic anomalies often exhibit a bright, negative amplitude top reflection against a generally lower amplitude background response (Fig. 5). The anomalies vary in their seismic character and have been subdivided into four categories:

Figure 6. A regional map of the area covered by 3D seismic data, displaying all seismic anomalies that were identified and interpreted to represent shallow hydrocarbon occurrences, the location of paleo-rift topography and the direction of glacial unit progradation. Location of Figures 7 and 11 are shown.

Figure 7. Enlarged section of the Pitu area shown in Figure 6 (A), displaying the seismic anomalies interpreted as shallow hydrocarbon occurrences from categories I and II. Category I anomalies are colour coded to match the key types of isolated anomalies shown within the adjacent seismic boxes (B, C and D). An example of category II anomalies, corresponding to the blue polygons in (A), is shown in box E. Seismic line locations of key examples (B-E) and Figures 5, 8A, 8B, and 12 are shown on the map (A).

Category I: Isolated anomalies

The majority of seismic anomalies observed across the study area occur as isolated, negative amplitude anomalies within a background of subtle or low amplitudes (Figs 6, 7 and 8). These isolated (category I) anomalies still vary in seismic character and therefore have been subdivided into four key types (Figs 5 and 7B-D; Type 1-4). The vast majority of category I anomalies display a small, bright event, characterized by a single loop trough-peak response (Type 1) (Fig. 5). These anomalies are limited in the horizontal (< ~150 m) and vertical (< ~20 m) plane but tend to occur at various stratigraphic levels (Figs. 5, 7B and 8). Polarity reversals are occasionally observed at the edge of the anomaly, dependent on the seismic properties of the host sediments.

Figure 8. Seismic cross sections, un-interpreted (left) and with interpretations (right), showing identified shallow seismic anomalies. (A) Seismic cross sections illustrating category I, II and IV seismic anomalies observed within the Pitu survey area. Dense faulting and hydrocarbon occurrences are shown throughout the sealing unit (mu-D1) of the Eocene reservoir. (B) Seismic cross sections highlighting category I anomalies within anticlinal folds. Category II (blue) and IV (yellow) anomalies are present in both profiles along with the gas hydrate stability zone (GHSZ) (blue dashed line), with the wide and thin dash representing high and low amplitude sections of the bottom simulating reflector (BSR) respectively. Seismic line locations are shown in Figure 7

Isolated anomalies also occur as larger features observed across multiple stratigraphic layers (horizontal/vertical extent of >2 km/>200 m) characterised by bright negative amplitude top reflections and a positive amplitude base (Type 2) (Figs. 5 and 7A). Internal reflections exhibiting bright amplitudes, as well as polarity reversals at the edge of the stacked anomalies, suggests a variable pore fluid as the main cause for the lower seismic velocities (Fig. 5).

Within mu-D1, above the southern extension of the MBR, a concentration of category I anomalies occurs (Type 3). These anomalies differ from the more typical Type 1, as they appear restricted to a single stratigraphic horizon, with the anomalies and the surrounding stratigraphy being offset by closely spaced, near vertical linear features characterised by dim amplitudes (Figs. 7 and 8A). These offsets are interpreted as small faults that extend downwards to the base of the Eocene gas reservoir (see category IV). A seismic variance attribute extraction through the stratigraphy at this depth shows a dense network of these

faults (Fig. 9A-B). The bright anomalies occur in between the faults suggesting entrapment of hydrocarbon fluids focussed within the Miocene interval directly above the MBR (Figs. 8 and 9A-B).

Figure 9. Seismic data illustrating the relationship between faults and hydrocarbon fluid signatures. (A) Time slice surface of seismic variance from the Pitu 3D survey (depth of 1336 TWT corresponding to mu-D1), displaying a concentrated network of small, high amplitude (variance) faults on the crest of the Melville Bay Ridge. The relationship between the location of small fluid anomalies observed within mu-D1 (yellow dashed areas) and the network of faults is shown. A minimum amplitude extraction displaying the location of the individual anomalies across a section of (A) is shown on (B), highlighting this relationship further. (C) A time slice of seismic variance from the Pitu 3D survey at a depth of -1178 TWT, showing the difference in the fault network at this shallower depth (compared to A). The location of the observed BSR and a minimum amplitude extraction displaying the location of fluid anomalies trapped beneath the GHSZ (category II) are shown. The locations of A and C are shown on Figure 3. (D) A seismic cross section in two-way-time from the Pitu 3D survey displaying potential fluid anomalies trapped within and truncated against a vertically extensive tectonic fault. This fault is observed to cross cut a low amplitude section of the bottom simulating reflector (BSR), which is also shown on (E). The location of both (D) and (E) is shown on (C).

Several, more laterally continuous faults are also observed on the variance extraction (Fig. 9), with some containing small, bright amplitude seismic anomalies within or truncating against the low amplitude linear zone between the offset horizons, a zone likely representing the fault plane (Figs. 8 and 9D).

Numerous category I anomalies are observed at the base of mu-C in a limited area in the southern part of the Pitu HR survey (Fig. 7A – purple polygons). These anomalies, referred to as Type 4, occur as vertically stacked, negative amplitude narrow anticlines across several layers of stratigraphy. The anticlinal anomalies follow the structure of the host stratigraphy, and often gradually diminishing upwards suggesting drape across an underlying structure (Figs. 7D and 8B). In the lower section of mu-C (Fig. 8B), the anomalies occur in between fault locations within the underlying and more chaotic section of mu-D. They also become more widespread (~2 km) above a local unit of enhanced thickness within mu-D1 (Fig. 8B), which causes the overlying anomalies and the surrounding stratigraphy to dip more steeply around its crest.

Category II: Anomalies terminating at the base GHSZ

This category refers to bright, negative amplitude anomalies observed within dipping strata packages that terminate at a level corresponding to a BSR (Figs. 7 and 10). The BSR appears as a cross-cutting negative amplitude reflection, interpreted as the base of the GHSZ (see section 4.2) (Figs. 10). These anomalies exist within multiple layers of tilted stratigraphy with the bright negative response existing for ~50 ms below the BSR (Fig. 8C). The brightest terminating anomalies exist within linear zones that trend northwest-southeast (Figs. 9C and 10C) and represent the location where the base GHSZ cross-cuts the host layers. These host layers maintain a bright reflection down-dip from the truncated anomaly, but switch to a positive amplitude response that continues regionally across the study area (Fig. 10A). The category II anomalies are most clearly expressed above laterally and vertically extensive faults that extend from the top horizon (e1) of the western flank of the MBR, to a near-seabed position (Figs. 2, 3, 9C and 10).

Figure 10. Bottom simulating reflectors (BSR) and gas hydrates. A) A composite seismic cross section from the Anu and Pitu 3D seismic surveys along part of the northern and southern

extensions of the Melville Bay Ridge as well as the deep valley between the two extensions. A discontinuous BSR can be observed above much of the paleo-rift structure, but is not observed above the majority of the valley area. The BSR varies in amplitude between areas containing terminating bright anomalies at the base gas hydrate stability zone (GHSZ) and areas without these anomalies where it displays as a low amplitude reflection (highlighted by white brackets). B) A seismic cross section in two-way-time from the Pitu HR 3D survey showing a clear cross-cutting BSR, as well as numerous bright anomalies terminating at the base of the GHSZ (category II). The location of both (A) and (B) are shown on (C). C) A minimum amplitude extraction for a 20 ms two-way-time window across the mapped BSR horizon that highlights the location of bright amplitude anomalies that terminate at the base of the GHSZ (category II). The relationship of the hydrate deposits to the underlying Melville Bay Ridge is also shown, via the underlying two-way-time structure map of horizon e1 defining the ridge topography. The intersection of a regional potentially porous horizon (identified on A) with the base GHSZ is also shown (yellow dashed line), with the intersection location coinciding with numerous terminating fluid anomalies.

Category III: Steeply dipping bright horizons

This anomaly category is observed within the progradational units of mu-A, forming part of the Melville Bay Trough Mouth Fan (Figs. 1, 2, 6 and 11) (Knutz et al., 2019). It is characterized by anomalously bright, negative amplitude top reflections, that display top set erosion and are interpreted as glacial clinoform packages (Fig. 11) (Newton et al., 2020). The clinoforms covered by the Anu 3D seismic survey display west to south-westerly dips (Figs. 6 and 11). The category III anomalies are distributed throughout much of the shallow stratigraphy (uppermost 1 second TWT) within the Anu 3D survey (light green area; Fig. 6), but with the highest amplitudes observed below the truncated top-sets, representing paleo-shelf breaks of the prograding wedge (dark green areas; Fig. 6). Towards the northwest within the survey area, corresponding to the oldest prograding units, dipping bright horizons terminate abruptly up-dip against a major glaciogenic unconformity (Fig. 11). Down-dip, the category III anomalies continue along semi-continuous, seismic-stratigraphic horizons but with variable and generally fading amplitudes (Fig. 11).

Figure 11. Uninterpreted and interpreted seismic cross section in two-way-time from the Anu 3D survey, highlighting steeply dipping bright horizons (category III) (yellow) from within the glacigenic stratigraphy of mu-A. Isolated shallow gas anomalies (category I) are also shown (red). The distribution of the category III anomalies and the location of the seismic intersection are shown on Figure 6.

Category IV: Eocene gas reservoir

An extensive, potential gas reservoir has been mapped at the base of the Cenozoic succession (mu-D2) overlying the MBR (Fig. 8) (Cox et al., 2020a). The reservoir is likely of Eocene age and interpreted as laterally continuous sand deposits on the northern parts of the ridge crest while towards the south and east, the unit appears fragmented due to mass transport (Figs. 8 and 12). Thus, large sections of the reservoir exist as separated blocks above a likely muddy decollement surface (represented by horizon e1) (Figs. 2 and 8). The reservoir package displays very bright amplitudes on seismic data including a bright negative amplitude top reflection and a bright positive amplitude base (Fig. 8a).

Figure 12. A two-way-time structure map of horizon e1 that represents the top of the Melville Bay Ridge overlaid by the distribution of the Eocene gas reservoir (category IV) across the ridge crest (black polygons) (Cox et al., 2020). The location of Isolated anomalies (category I) (red polygons), interpreted to represent shallow gas, are shown with their distribution following the trend of the underlying reservoir. This spatial relationship may suggest that the deeper reservoir is leaking hydrocarbons into the overlying stratigraphy.

The thin overlying sealing stratigraphy of mu-D1 is characterised by a dense network of closely spaced small offset faults that often appear aligned to the edge of the reservoir blocks (Figs. 8 and 9A-B). These faults, hosting isolated bright anomalies (category I), commonly extend between the base of the reservoir (horizon e1) and horizon d1, with some extending upwards towards the seabed. Hence, there is a clear spatial relationship between the regional distribution of the reservoir blocks on the MBR crest and the isolated anomalies throughout the shallow stratigraphy (mu-D1 and -C) (Figs. 6 and 12).

4.2 Gas Hydrates

A discontinuous BSR has been observed across an area of 537 km² above the central axis and western flank of the MBR (Figs. 6, 7 and 10). This feature exists approximately 200 m below

the seafloor, in water depths of 625–720 m and marks the base of the GHSZ. The BSR is observed as a negative amplitude reflection with variable intensity that cross-cuts the stratigraphy. It is best defined in areas with tilted stratigraphy where bright anomalies terminate at the BSR and the base of the GHSZ (category II) (Figs. 7E and 10B). Away from these anomalies, and especially in areas where the stratigraphic dip is similar to the seabed the BSR amplitude is reduced to a dimmer response, but can still be observed (Figs. 8, 9D-E and 10).

The seafloor topography across the region contains several erosional and depositional features related to glaciation (Figs. 1 and 14). The BSR is observed to mirror this seafloor topography, deepening and shallowing in areas of erosion and deposition, respectively – e.g. such as the glacial wedge (Figs. 10A and 13G-H). The thickness of the GHSZ varies, generally in relation to seabed depth – e.g. with the GHSZ thinning or thickening in areas of shallower or deeper water, respectively. An exception to this trend is observed in the northern and eastern parts of the BSR, where the GHSZ thins in areas where water depth increases (Fig. 13C and E). The increased water depths are a result of seabed glacial erosion (Fig. 14) (Newton et al., 2017).

Interval velocities increase by ~200 m/s within the stratigraphy above the BSR (e.g. GHSZ), when compared with areas outside the BSR (Fig. 4). Below the BSR, seismic velocities at the GHSZ base are reduced from ~2200 m/s within the GHSZ to ~1800-1900 m/s beneath. Conversely, a velocity increase is observed at a corresponding depth level away from the BSR (Fig. 4).

Despite its discontinuous appearance, the distribution of the BSR suggests a relationship to the paleo-rift topography and the MBR. The BSR is observed in most areas along the western flank of the MBR, but disappears above a deep valley between the northern and southern extensions of the ridge (Fig. 10A). In the vicinity of the valley system, the amplitude strength of the BSR reduces, and disappears completely above the central parts of the valley. Within the buried valley zone, several of the regional horizons that host the bright category II anomalies are located at depths well below the depth of the base GHSZ. The lack of cross-cutting between the host strata and the GHSZ within this area is a likely reducing factor for the seismic imaging of the BSR (Fig. 10A and C). In areas containing extensive faults that extend from the top ridge horizon (horizon e1) and through the post-rift stratigraphy, the BSR retains a strong amplitude response within the host strata (Figs. 2, 3, 9C and 10).

Figure 13. Maps showing the calculated average geothermal gradient (A) and average heat flow (B) through the gas hydrate stability zone (GHSZ) interval for the area containing the observed bottom simulating reflector (BSR) within the Pitu depth survey limits. Maps used within this calculation are shown including seabed depth (C), BSR depth, pressure and temperature (D), GHSZ thickness (E) and average interval velocity through the GHSZ (F). Seismic cross sections in two-way-time (G) and depth (H) are shown across a section within the south of the BSR distribution highlighting the irregular seabed topography, and the likely post-glacial re-equilibration of the hydrate phase boundary beneath a depositional glacial wedge.

4.3 Evidence for Seabed Fluid Escape

The seafloor located in the northern part of the study area represents a major glacial trough, characterised by numerous features of glacial erosion and deposition, such as lineations, ridges, iceberg scours and grounding zone wedges (GZW) (Figs. 2, 13 and 14) (Newton et al., 2017). Within the trough area, semi-circular seafloor depressions are commonly observed, with lateral dimensions up to 500 m and depths up to 50 m (Fig. 14D-B). Small mounds of sediment often occur on the seabed next to the depression. These mounds are not evenly distributed but tend to be skewed to one side of the depression (Fig. 14D).

Figure 14. Seabed Mapping. A) A two-way-time structure map of the seabed horizon across the area of 3D seismic coverage, highlighting the widespread distribution of glacial-erosional and depositional features. Numerous curvilinear and concentric seabed depressions are observed on both a seismic cross section in two-way-time (B) and the seabed surface (C), basinward of a grounding zone wedge (GZW) (Newton et al., 2017). The dashed white line on (B) represents the base of the GZW. Similar features are observed within the Pitu survey area on both the seabed surface (D) and in seismic cross section (E). (F) An amplitude map of the seabed horizon across the 3D seismic coverage that displays the relationship between glacial erosion and depositional features on the seabed and seismic amplitude.

The depressions seem to be unrelated to the underlying stratigraphy, as no seismic features are observed consistently beneath their locations, such as faults, pipes or anomalous brightening (although on occasion a fault will occur beneath the depression, e.g. Fig. 14E). On the seabed structure map, curvilinear scours are often observed connecting the circular depressions, commonly extending towards the northeast, trending similar to glacial lineations (Fig. 14B and D). In the western part of the study area (Anu survey), numerous seabed depressions occur towards the southwest, lee-side of a depositional feature interpreted as a GZW (Newton et al., 2017). Several semi-circular depressions are also observed on the base horizon of the GZW, which represents a paleo-seabed surface (white dashed line on Fig. 14C). Both the seabed depressions and GZW deposits coincide with lower seismic amplitudes of the seabed horizon (Fig. 14E). Based on seabed geomorphology and the distribution of glacial features, the semi-circular depressions are interpreted as having been formed by glacial erosion, and most likely represent iceberg pit-marks (e.g. Brown et al., 2017) as opposed to gas-hydrate explosion craters (e.g. Andreassen et al., 2017).

4.4 Geothermal Gradient

The geothermal gradient has been estimated using the GHSZ thickness inferred from the BSR distribution covered by the Pitu 3D survey (depth domain) and known P-T phase relationships for gas hydrates (Fig. 13; section 3.3). Accordingly, pressure and temperature at the BSR

depth, range between 8.0 - 9.5 MPa (average 8.9), and 10.0 - 11.6 °C (average 10.9) respectively (Fig. 13D). As both the pressure and temperature estimations are dependent on BSR depth, the two parameters show identical lateral variation. Hence, shallowing of the BSR coinciding with a shallowing seabed depth, as seen in the southern part of the Pitu survey (in the area of glaciogenic deposition), causes a reduction in both pressure and temperature (Fig. 13). A differing trend to that of the seabed depth is seen in the northern section and along the eastern edge where the seabed deepens, at the same locations where the relationship between seabed depth and GHSZ thickness diverts (section 4.2).

The calculated geothermal gradient across the thickness of the GHSZ ranges from 40 - 59 °C/km with an average of 49 °C/km (Fig. 13). The trend of the estimated geothermal gradient matches that of the GHSZ thickness, with the geothermal gradient increasing in areas of a thinner stability zone and vice versa. However, superimposed on this trend, are a number of localised high values that are either concentric or linear in shape. These anomalous values occur in the same location as similar features observed on both the GHSZ thickness (Fig. 13E) and the seabed depth maps (Fig. 13C).

The interval velocities through the GHSZ range between 1950-2350 m/s (Fig. 13F) and are observed to increase towards the south within an area coinciding with glaciogenic deposition at the seabed (Fig. 14 C, and F-H). The conversion of these velocities to thermal conductivity yields a range from 1.45 to 1.85 W/m⁻¹/K⁻¹. The thermal conductivity estimates, in combination with the geothermal gradient model values, produces a heat flow across the thickness of the GHSZ, ranging from 58 - 100 mW/m² with an average of 81 mW/m² (Fig. 13B). Again, several concentric or linear anomalies are observed on the heat flow map (Fig. 13B), which coincide with areas of high geothermal gradient, a thin GHSZ and high interval velocities.

5. Discussion

5.1 Hydrocarbon Occurrence

The detailed analysis of the shallow Cenozoic stratigraphy in Melville Bay yielded numerous seismic amplitude anomalies which have been interpreted to represent the most northerly occurrence of shallow gas and gas hydrates offshore western Greenland (Figs. 6-8 and 11). The gas anomalies were categorised by seismic character and mainly represent the different trapping mechanisms observed across the region (categories I-IV), with the majority of hydrocarbon occurrences existing as isolated pockets of gas (category I), with variable seismic character (Type 1-4) (Figs. 5-9).

Free gas was observed trapped against the base of the GHSZ (category II) (Figs. 6-10), a boundary recognised by a discontinuous BSR (Berndt et al., 2004; Hillman et al., 2017), hosted within tilted, likely porous horizons, with the termination of the fluid response down dip (Fig. 10B), suggesting a maximum gas column of ~50 m. Dimming of the BSR (Figs. 8, 9D, 9E and 10) occurs in areas away from these terminating free gas anomalies, as the acoustic impedance contrast at the base GHSZ is lowered (Hilterman, 2001). The free gas may be absent due to a lack of migration, lack of reservoir at the base GHSZ, and due to all available gas having been converted to hydrate. The dimming may suggest low saturation of gas hydrate in areas without a BSR (Spence et al., 1995). It is also possible that dim or absent BSRs could be a result of recent glaciations having caused variations in the temperature field which still persist today, if the hydrate system has not fully re-equilibrated post-glaciation (Crémière et al., 2016; Grassmann et al., 2010; Mienert et al., 2000). Overall, the abrupt alternations between BSR

and no BSR seen in Fig. 10 are probably due to a combination of stratigraphic occurrence of reservoir porosity and permeability and availability of methane around the base of the GHSZ. Furthermore, the gas interpreted to exist within glacigenic, progradational units of mu-A (category III) (Knutz et al., 2019), is observed trapped up-dip against horizontal and unconformable muddy strata of the overlying glacial sequence (Fig. 11). The brightest fluid-related amplitudes coincide with truncated top-sets at the paleo-shelf break positions of the prograding wedge; possibly representing increased gas concentrations or greater porosities (Hilterman, 2001). The rotating alignment of these fluid anomalies southward, as well as the variable dip of glacigenic stratigraphy (Fig. 6), reflects the variable pathways of ice streams and shelf break progradation (Knutz et al., 2019; Newton et al., 2020; 2017).

5.2 Fluid Migration

Although the seismic evidence provided only offers a static view of contemporary hydrocarbon occurrences, and features such as chimneys, pipes and pockmarks are not observed at present day (Chand et al., 2012; Huuse et al., 2010), several relationships between structural and stratigraphic elements and the distribution and character of the hydrocarbons observed, provides evidence towards understanding the migration history of fluids within this area.

Paleo-rift topography and tectonic faults

A significant concentration of free gas anomalies, as well as all identified gas hydrate deposits, exist directly above or along the western flank of the underlying MBR (Figs. 6-7, 9-10 and 12), with the deposits only becoming discontinuous above a large buried valley separating the ridge's north and south extensions (Fig. 6 and 10). This relationship suggests that the underlying paleo-rift topography is influencing upward fluid migration. Post-rift depositional units either onlap onto the ridge flanks, or extend and thin above its crest, forming a broad anticline structure throughout mu-D and -C (Fig. 2) (Gregersen et al., 2019; 2013). This causes the post-rift stratigraphy within the adjacent grabens to tilt towards the ridge structure, likely facilitating the up-dip migration of fluids into areas above the MBR.

Potential Cretaceous source rock intervals within mu-F (Nohr-Hansen et al., 2018; Planke et al., 2009), are interpreted to extend from the Melville Bay Graben up-dip into the MBR structure on the eastern flank; a factor which likely led to the charging of the Eocene reservoir (category IV) (Cox et al., 2020a). On the western flank the syn-rift stratigraphy terminates against deep tectonic faults (Figs. 2, 3 and 15), with disconnection of this strata occurring at the western ridge fault. This termination and offset likely restricts fluid migration from the South Kivioq Basin, and instead, fluids are forced upward through a number of post-rift fault conduits that are observed to extend from the tips of deeper faults and the top ridge horizon (horizon e1), to close to the seabed (Fig. 2-3, 9 and 15). Above these faults on the western ridge flank, gas hydrate deposits (Figs. 6, 9-10) suggest the location of these migration pathways have influenced gas hydrate formation.

Figure 15. A composite seismic cross section in two-way-time across the Anu and Pitu 3D seismic surveys, overlain by an interpretation of the structure, stratigraphy and complex fluid migration history that likely characterises the study area. Fluid migration into the Cenozoic stratigraphy is observed via syn-rift carrier beds and tectonic faults from both within the ridge and above its western flank. The location of shallow gas accumulations, the Eocene gas reservoir and gas hydrate deposits, along with the potential migration pathways for these fluids is shown, along with possible effects of glaciation on hydrocarbon remigration. The location of the seismic line is shown on Figure 3.

Furthermore, free gas trapped beneath the hydrate deposits (category II) is also observed above these fault locations (Fig. 9C), although this distribution may instead be influenced by the intersection of the host strata (regional, potentially porous and permeable horizons), that have been uplifted and tilted by the MBR structure, with the base GHSZ along the western flank of the ridge (Figs. 9C, 10 and 15). Still, no free gas is observed within the GHSZ above the fault locations (Fig. 10 and 15) and no seabed expulsion features are observed directly above the fault tips (Fig. 10 and 14-15). Therefore, any fluids migrating upward through the faults, post hydrate formation, either became trapped within the fault plane at the base GHSZ (Fig. 15), or migrated stratigraphically up-dip once reaching the potentially porous carrier bed horizons until again becoming trapped at the base GHSZ (Figs. 10 and 15).

Reservoir Leakage

Above the crest of the MBR, a clear relationship is observed between the location of isolated gas anomalies (category I) and the trend of the Eocene gas reservoir (category IV) (Fig. 6, 8 and 12). The sealing unit (mu-D1) is at its thinnest above the reservoir (due to depositional thinning above the ridge and erosion) (Cox et al., 2020a; Gregersen et al., 2013), and is observed to contain a dense network of short offset, near vertical faults, extending from the base of the reservoir (horizon e1) to the top of the sealing unit (horizon d1) (Cox et al., 2020a).

Several fluid anomalies are observed trapped within this dense network of faults (Figs. 8A and 9A-B), with their occurrence, as well as overlying anomalies in the lower section of mu-C (Figs. 8A, 10A and 12), suggesting that the underlying reservoir is leaking hydrocarbons upwards through these fault conduits (Fig. 8-9, 12 and 15) (Cartwright et al., 2007; Ingram and Urai, 1999).

These faults occur in a dense, polygonal network (Figs. 3 and 8-9) and are geometrically similar to sets of polygonal faults within the same stratigraphy above the grabens (Figs. 2 and 15) (Cartwright and Dewhurst, 1998; Cox et al., 2020a). However, their exact origin is uncertain and fault growth in certain areas may instead be controlled by the presence of the underlying deformed reservoir (Figs. 8B and 12), with normal faults forming along the flanks of reservoir blocks, likely due to differential compaction above the blocks and adjacent areas (Fig. 8) (Cox et al., 2020a). Polygonal faults are then thought to nucleate at the tip of these faults (at horizon d1) and extend vertically into mu-C. A similar scenario may have occurred above the ridge crest, where the gas anomalies are observed (Figs. 8-9). Here, the underlying reservoir is more laterally continuous, but faults may still be influenced by reservoir structure as they coincide with irregular offsets between narrow sections of the reservoir (Fig. 8A), although this offset may instead be caused by the faults themselves. Therefore, if fault genesis is not typically polygonal (Cartwright et al., 2003), then gas leakage through these faults is more likely as polygonally faulted muds are known to create excellent sealing formations (Cartwright, 2019; Goult, 2008). If leaking did occur, then this may be providing at least part of the methane constituent of the overlying hydrate deposits (Figs. 7-10).

Glacial clinoforms

The source and likely migration pathway of the gas interpreted to exist within glacial clinoform units of mu-A (category III) (Figs. 2 and 11) is uncertain, due to the disconnection of this stratigraphy from potential source rock horizons in the deeper basins (Fig. 2) (Cox et al., 2020a; Nohr-Hansen et al., 2018) via thick packages of likely sealing formations including hemipelagic muds (mu-D) and contourites (mu-C and -B) (Gregersen et al., 2013; Knutz et al., 2015). No deep tectonic fault connections are observed, and the paleo-rift topography close to the shelf edge (Figs. 1 and 2) is likely too far away to focus fluids into sediments that were only deposited since ~2.7 Ma (Knutz et al., 2019). Shallow source rocks may exist, although sufficient burial and time for maturation is unlikely when considering burial only increased after ~2.7 Ma (Knutz et al., 2019; Wilson, 1975). Instead, the gas could be biogenically generated, either in situ as the clinoforms may contain organic material - as suggested for other glacial related clinoforms, e.g. Verweij et al. (2012); Muller et al. (2018) – or more likely, from organic horizons within the contourite succession, e.g. Knapp et al. (2019); Rebesco et al. (2014). The contourites (mu-C and -B) are estimated to exist at temperatures around 40-50 °C at present day (Fig. 11), the theoretical peak temperature of biogenic generation (Stopler et al., 2014), based on the estimated shallow geothermal gradient from this study (49 °C/km) (Fig. 13).

Seabed expulsion

Attempts were made to document fluid expulsion features at the seabed (e.g. chimneys, pipes and pockmarks) which may represent the existence of cold hydrocarbon seeps into the water column (Andreassen et al., 2017; Chand et al., 2012), similar to those observed ~500 km to the south near Disko Island (Nielsen et al., 2014). The seafloor across the study area, however, represents a time-transgressive glacial unconformity that has experienced significant erosion since ~2.7 Ma (Figs. 2 and 14) (Bennett et al., 2014; Knutz et al., 2019; Newton et al., 2020). This erosion has removed large amounts of sediment from the inner shelf and likely removed

any seabed expulsion features that may have formed prior to glaciation (Fig. 14). Further towards the shelf edge, horizons interpreted as pre-glacial paleo-seabeds are now buried beneath a thick unit of glacial sedimentation (Fig. 2), and seismic resolution is likely insufficient to distinctly image any potential buried features. Additionally, much of the area above the MBR, where upward fluid migration is focussed, contains gas hydrates (Figs. 2, 6-7, 10 and 15), which may restrict upward fluid migration and expulsion to the surface (through both conventional trapping - such as the free gas anomalies observed - and transformation to hydrate) (Grauls, 2001; White, 1979).

Several erosional depressions are however, observed on the present day seabed within two distinct regions of the 3D data (Fig. 14). These features could represent fluid escape locations at the seabed (Andreassen et al., 2017; Chand et al., 2012), but no direct evidence for fluid flow is observed, although features such as gas chimneys would likely have had time to dissipate if formed during the early stages of glaciation (Huuse et al., 2010). Evidence such as their geometry, the asymmetrical sediment berms and their occurrence within seabed scours (Fig. 14), instead suggests that the depressions are more likely associated with glacial erosion of the seabed, and are interpreted as iceberg pit-marks (Brown et al., 2017). Such pits form by the impact of an iceberg keel with the seabed (Newton et al., 2018; Woodworth-Lynas et al., 1985), with the adjacent asymmetrical berms of sediment (Fig. 14E) likely having been excavated and deposited to one side by the iceberg upon impact. The connection of several of the depressions by curvilinear scours (Fig. 14B and D), marking the iceberg pathway across the seafloor in between low tides, strongly supports genesis by iceberg grounding (Brown et al., 2017; Newton et al., 2016). Furthermore, the depressions within the Anu survey were observed basinward of a major grounding zone wedge (Fig. 14B and C), marking a potential ice sheet calving margin (Newton et al., 2020; 2017). Icebergs reworking the seafloor have been observed in water depths up to, and occasionally exceeding, 1 km offshore Greenland, e.g. Kuijpers et al. (2007), meaning that icebergs impacting the seafloor in the observed water depths of ~650 m is not uncommon.

5.3 Geothermal Gradient and Heat Flow

Geothermal gradient and heat flow estimations from this study provide the only data points across the entire continental shelf of western Greenland (Lucazeau, 2019). An average shallow geothermal gradient of 49 °C/km and heat flow of 70-90 mW/m² was estimated (Fig. 13), with these values being comparatively high when compared to the closest available (~225 km away from the study area) temperature probe data from within the centre of Baffin Bay (but only for the top <~2 m of sediment), which recorded five geothermal gradient values between 26-48 °C/km and heat flow values between 54-64 mW/m² (Lucazeau, 2019; Pye and Hyndman, 1972). The heat flow estimate is also slightly greater than the nearest points (64-75 mW/m²) in the global heat flow model by Davies (2013), albeit at the edge of its interpolated coverage. Several factors may have resulted in higher geothermal gradient and heat flow estimations (Fig. 13). This could be associated with uncertainty in both the BSR based estimation method (up to ~50-60%; Grevemeyer and Villinger, (2001); see section 3.3) and the temperature probe measurements of which the data are compared (Pye and Hyndman, 1972). An increase in heat flow is expected however, in areas of focussed fluid flow (Ganguly et al., 2000; Minshull and Keddle, 2010), such as above the MBR, and also due to the advection of heat towards underlying paleo-rift topography (the MBR) (Serié et al., 2017). Hydrocarbon leakage from the underlying Eocene gas reservoir may also add to this effect (Figs. 8-9 and 12). Heat flow may have been over estimated however, due to the use of seismic interval velocities to derive thermal conductivity (see section 3.3). The velocity within the GHSZ has likely been elevated by the presence of gas hydrate (Fig. 4) (Shankar and Riedel, 2011; Stoll et al., 1971), as such

rapid lateral variations in velocity are unlikely to be geological. The thermal conductivity of methane hydrate is approximately equal to the pore water (<10% difference) (Ruppel, 2000; Waite et al., 2009), so elevated velocity would cause an over estimation of both thermal conductivity and heat flow, and the results may in fact be closer to those estimated previously (Lucazeau, 2019; Pye and Hyndman, 1972). Additionally, heat flow may not be in a steady state, due to the impact of recent glaciations on the temperature regime (Johansen et al., 1996), such as is observed on the Norwegian margin (Jung and Vogt, 2004; Mienert et al., 2000). Therefore, the hydrate system may not yet have fully re-equilibrated post-glaciation, affecting the BSR depth and heat flow estimates (see section 5.4).

Several localised, high geothermal gradient and heat flow anomalies are observed across the BSR area (Fig. 13), but no seismic features, that may suggest focussed fluid flow pathways (e.g. pipes or faults), are observed beneath (Ganguly et al., 2000; Minshull and Keddle, 2010). Instead, many of the anomalies coincide with either positive, likely depositional, or negative, erosional seabed features that likely formed during the last glaciation (Figs. 13-14) (Newton et al., 2020; 2017). These include multiple concentric and linear anomalies that represent iceberg pit-marks, glacial lineations and shallow seabed depressions (Fig. 13). These erosional features have caused localised deepening of the seabed, which is not reflected at the BSR depth (or at least is not visible given the seismic resolution), causing a thinner GHSZ, and increased apparent geothermal gradients (Fig. 13A and E).

5.4 Possible Impacts of Glaciation

Melville Bay has experienced multiple cycles of ice sheet advance and retreat across the shelf since ~2.7 Ma (Knutz et al., 2019), resulting in the removal of vast amounts of sediment from the inner shelf and the re-deposition of this sediment to the shelf edge, as part of the Melville Bay Trough Mouth Fan (mu-A) (Figs. 1-2, 11 and 15) (Knutz et al., 2019; Newton et al., 2020). These processes have transformed the structural position of the stratigraphy across the shelf (Fig. 2), with structural changes likely exacerbated by isostatic compensation resulting from load redistribution (Fjeldskaar and Amantov, 2018; Zieba and Grover, 2016). The combination of erosion from the inner shelf and the increased burial (and compaction) of post-rift sediments beneath the glacial wedge on the outer shelf (Fig. 2), as well as isostatic compensation, has led to the Melville Bay margin tilting basinward west of the MBR. Tilting of the stratigraphy has likely effected fluid migration by focussing fluids up-dip towards the inner shelf and above the MBR, possibly contributing to increased hydrocarbon occurrences in this area (Figs. 2, 6-7 and 15).

Long-term sediment redistribution and tilting likely occurred alongside repeated cycles of glacial loading on the shelf, impacting both isostasy and subsurface conditions (Cavanagh et al., 2006; Medvedev et al., 2019; Ostanin et al., 2017). Cyclic fluctuations in subsurface pressure and temperature during glacial-interglacial cycles, may have promoted fluid remigration (Fig. 15) (Goffey et al., 2016; Plaza-Faverola et al., 2011), with increased pore pressure beneath the ice load, potentially causing the fracturing of hydrocarbon seals and leakage (Hermanrud and Nordgard Bolas, 2002; Tasianan et al., 2018). This process may explain the dense network of fractures and gas pockets observed within the Eocene gas reservoir seal (mu-D1) and the overlying stratigraphy (Figs. 8-9). Furthermore, faults may reactivate, increasing fault permeability during deglaciation and load removal (Løtveit et al., 2011; Ostanin et al., 2017), possibly promoting leakage through the mu-D1 fractures, and increasing fluid migration through larger syn- and post-rift faults parallel to the MBR. This may have contributed to the increase in hydrocarbon occurrences (Figs. 6-8 and 12) and the formation of gas hydrates (Figs. 10 and 15) above the western flank of the MBR.

Glacial-related variations in subsurface conditions can also affect the stability of gas hydrate (Portnov et al., 2016). The relatively large water depths in the study area (~650 m) mean the seabed is well within the stable region of the gas hydrate phase diagram (Fig. 16) and can thus be considered relatively stable, with hydrate dissociation at the seabed only likely to occur in response to glacial erosion (unlike that seen at shallower water depths in the Barents Sea, e.g. Andreassen et al., 2017). These variations are more likely to have affected hydrate formation and dissociation at the phase boundary at the base of the GHSZ (Fig. 16) (Ruppel and Kessler, 2017; Serov et al., 2017). Ice loading and erosion during glacial periods likely cooled the underlying sediments and increased pore pressure, allowing increased hydrate stability and a deeper phase boundary than during ice-free periods (Fig. 16) (Grassmann et al., 2010; Ostanin et al., 2017). This suggests gas hydrate may have expanded downwards during glacial periods and once deglaciation and load removal began, would have experienced hydrate dissociation at the base of the stability zone (Portnov et al., 2016; Serov et al., 2017). This process may have contributed to the numerous free gas accumulations that are observed trapped at the base of the present day GHSZ (Figs. 6-10).

Post-glacial re-equilibration and shallowing of the phase boundary is evidenced beneath a glaciogenic wedge (Figs. 10A and 13), where the BSR has shallowed significantly and mirrors the post-glacial seabed topography. However, evidence for the phase boundary not yet having re-equilibrated post-glaciation is observed below an area of recent glacial-related seabed erosion (evidenced by glacial lineations) (Fig. 13C and 14) (Milkov and Sassen, 2000; Wang et al., 2006). This is causing an un-expectedly thin GHSZ in an area of deeper water (Fig. 13C and E) and has likely increased geothermal gradient and heat flow estimates (Fig. 13).

Figure 16. Temperature pressure conditions and methane hydrate stability. The phase boundary represents the transition of stable gas hydrate to free gas via dissociation and is based on the empirical relationship between pressure and dissociation temperature from Dickens and Quinby-Hunt (1994). Present day hydrate stability is shown at a seabed depth of 650 m and the present water temperature of 1.5 °C, with the estimated geothermal gradient through the gas hydrate stability zone (GHSZ) indicating the depth of the phase boundary and the observed bottom simulating reflector (BSR). Gas hydrate stability at the seabed is also shown to be less sensitive to future climate warming scenarios (3 °C increase in water bottom temperature in Baffin Bay) due to the relatively large water depths.

The sensitivity of the gas hydrate deposits to future climate warming is an important consideration, especially within the Arctic, which is an area sensitive to the amplification of temperature increases compared to lower latitudes (Serreze et al., 2000; Serreze and Barry,

2011). Bottom water temperatures in Baffin Bay are estimated to increase by 0.2 to 3 °C by 2100 in a response to global warming (Stocker et al., 2014). However, due to the hydrate stability imparted by the relatively deep, and cold waters in Melville Bay, the gas hydrate deposits documented here are, at least in the short-term, likely less sensitive to projected future warming scenarios than hydrates in shallower waters, such as the Barents Sea (Andreassen et al., 2017). Even at the maximum of the estimated warming (3 °C warmer ocean bottom temperatures), hydrate at the seabed is likely to remain stable (Fig. 16). This scenario would cause the hydrate phase boundary to shallow by ~50 m causing further dissociation at the base GHSZ. But for gas hydrate to dissociate at the seabed and be released into the atmosphere, ocean bottom water temperature would likely need to increase by ~8 °C, a scenario that is currently unlikely.

6. Conclusions

Numerous fluid related anomalies have been identified and mapped throughout the Cenozoic sedimentary succession of the Melville Bay continental shelf margin, using extensive 3D seismic data coverage. These data provide the most widespread and high-resolution imaging of the subsurface along the west coast of Greenland and the identified fluid anomalies represent the most northerly recorded occurrence of shallow gas and gas hydrates in Baffin Bay. Shallow gas anomalies have been categorized by different trapping styles, with free gas occurring in isolated pockets (category I), trapped at the base of the gas hydrate stability zone (GHSZ) (II), within laterally extensive glacial clinoforms (III) and finally within an Eocene aged, giant mass transport deposit reservoir (IV). Extensive gas hydrate deposits have been identified across an area of 537 km² via the identification of a discontinuous bottom simulating reflector (BSR) that represents the base of the GHSZ. The BSR was used to estimate a near surface geothermal gradient of 49 °C/km across the GHSZ and a heat flow of 70-90 mW/m², providing the first geothermal gradient and heat flow data points on the entire west Greenland margin.

Paleo-rift topography is predicted to have influenced fluid migration and the thermal regime, with increased concentrations of gas and all gas hydrate deposits occurring above the centre and western flank of the Melville Bay Ridge (MBR). Regional post-rift stratigraphy onlaps and is tilted towards the ridge, promoting fluid migration towards the ridge crest. Related sets of faults along the ridge flanks have likely provided fluid migration pathways from potential deeply buried Cretaceous source rocks towards the overlying Cenozoic stratigraphy. Leakage from the Eocene reservoir is also likely, evidenced by condensed gas anomalies both within and above the densely faulted overlying seal.

Multiple cycles of glaciation since ~2.7 Ma have likely affected the contemporary distribution of hydrocarbons and the fluid migration history. Extensive sediment redistribution from the inner to outer shelf, along with the resulting isostatic compensation, has caused a regional tilt of the margin basinward, focussing fluids up-dip towards the inner shelf and above the ridge. Variations in subsurface conditions due to repeated cycles of glacial (un)loading, have likely promoted fluid flow, potentially causing seal breach and leakage from the Eocene reservoir due to increased pore pressures, as well as increased migration through ridge flanking faults due to fault reactivation. Finally, variations in pressure and temperature likely led to the expansion of gas hydrate deposits during glacial periods, and subsequent hydrate dissociation at the phase boundary during deglaciation; a process which may have contributed to the numerous free gas accumulations observed at the base GHSZ at present day. The relatively large water depths in this gas hydrate province would probably ensure continued stability of the top of the GHSZ both during de-glaciation in the past and during most future warming scenarios over the next several decades.

Data Availability

The seismic data used within this study were kindly provided by Cairn Energy PLC (Pitu), Shell (Anu) and TGS (Regional 2D). To access these data, the respective company or the Greenland authorities (MLSA) will need to be contacted directly.

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