Retrieval of the Skin Sea Surface Temperature Using Hyperspectral Measurements From the Marine-Atmospheric Emitted Radiance Interferometer

Elizabeth Wong
University of Miami, ewong@rsmas.miami.edu

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RETRIEVAL OF THE SKIN SEA SURFACE TEMPERATURE USING HYPERSPECTRAL MEASUREMENTS FROM THE MARINE-ATMOSPHERIC EMITTED RADIANCE INTERFEROMETER

By

Elizabeth Wong

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Elizabeth Wong

Approved:

P.J. Minnett, Ph.D.
Professor of Meteorology &
Physical Oceanography

M. Brian Blake, Ph.D.
Dean of the Graduate School

M.G. Brown, Ph.D.
Professor of Applied
Marine Physics

G. Szczodrak, Ph.D.
Associate Scientist of
Meteorology & Physical
Oceanography
This dissertation document details research into the vertical profiles of temperature through the electromagnetic and thermal skin layers of the ocean. The Marine-Atmospheric Emitted Radiance Interferometer (M-AERI) is utilized to provide highly accurate, spectrally resolved radiance measurements in the infrared regime which, in turn, are used for the sensing of temperature values within the thermal skin layer depths of less than 1 mm. The inversion equation applied to the high resolution spectra is known to be non-linear and ill-conditioned. To constrain the solution and reduce the errors in this ill-conditioned retrieval problem, the truncated singular value decomposition (TSVD) regularization technique is adopted. The TSVD was first performed on synthetic data to assess the feasibility of the technique and subsequently on field datasets obtained from the M-AERI in which the errors associated with the use of this retrieval method were characterized. An averaged field of 300 spectra showed a vertical temperature inversion which was deemed unphysical by comparison with the solutions obtained from synthetic data runs and by a scaling analysis using the Rayleigh number. The inversion was removed by incrementing the sub-skin temperature of the first-guess profile required in the TSVD method as synthetic data results showed that the resulting profile converges to the surface and sub-skin temperature. Application of the technique to field data required
an additional step of averaging the radiance spectrum into 11 wavenumber intervals so that the problem would not be over-constrained. This was established by adding noise to synthetic data and observing the high variability in the retrieved brightness temperature values.
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Chapter 1

Introduction

The study of sea surface temperatures (SST) is an important area of research as it is one of the most widely used parameter in climate and ocean studies, particularly in its influence on air-sea interactions. SST is one of the main drivers in turbulent heat exchanges, gas and momentum transfers and various climate processes. Ohring et al. (2005) and the Interim Sea Surface Temperature Science Team, ISSTST (2010) stated that SSTs with an absolute accuracy of $< 0.1 \, K$ and a stability of $< 0.04 \, K$/decade for satellite-derived SST products are desired for large temporal and spatial studies for use in making accurate projections of climate change. Furthermore, Fairall et al. (1996b) have shown that accuracies of $10 \, Wm^{-2}$ in heat balance estimations requires an SST accuracy of $\pm 0.2 \, K$ and ideally the SST value should be the temperature measured exactly at the air-sea interface when bulk aerodynamic flux algorithms are used as they are developed for the computation of ocean fluxes occurring at the air-sea interface. Current satellite-derived SST values have accuracies of $\sim 0.33 \, K$ as in the case of the Advanced Very High Resolution Radiometer (AVHRR) (Kearns et al., 2000) and $\sim 0.23 \, K$ for the Advanced Along Track Scanning Radiometer (AATSR) (Embury
et al., 2012). The 0.1 K SST accuracy goal calls for highly accurate satellite correction algorithms and a much-needed deeper understanding of the physics behind the SST variable. In particular, the thermal skin SST layer is of interest as the heat for the energy fluxes happening directly at the air-sea interface is provided primarily by molecular processes which are the dominant causes of the thermal skin layer (Schluesselel et al., 1990).

Figure 1.1 shows a conceptual temperature versus depth profile of the ocean’s near-surface layer. The thermal skin layer, or cool-skin layer, is the layer of about a tenth of a millimeter thickness at the surface of the ocean. The surface temperature is cooler than the temperature just below by a value ranging from $\sim 0.1 \, ^\circ C$ during high wind speeds to $\sim 0.6 \, ^\circ C$ during low wind conditions (Ward, 2006). This seemingly unconventional temperature gradient in the thermal skin layer in which the lower layers are warmer than the upper surface layers occurs because the direction of heat fluxes is mainly from the ocean to the atmosphere. Heat loss by infrared (IR) radiation, latent heat, and sensible heat takes place at the interfacial layer of the ocean and results in the ocean releasing heat to the atmosphere rather than the reverse. Thus, the temperature gradient in the thermal skin layer is of great interest since the thermal skin layer is where most, if not all, of the ocean’s thermal energy is transferred into the atmosphere and may play a key thermodynamic role in the warming of the ocean by greenhouse gases (i.e. not the kinetic energy of currents and eddies).
Figure 1.1: Idealized temperature profiles of the near-surface layer (~10-m depth) of the ocean during nighttime or daytime during strong wind conditions (red curve) and daytime low wind speed and high insolation conditions resulting in thermal stratification of the surface layers (black curve). GHRSST (2012).

There are two skin layers at the ocean surface: the thermal skin layer and the electromagnetic (EM) skin layer. The thermal skin layer, also known as the molecular sub-layer, has a temperature gradient which is sustained by molecular conduction which supplies energy through the aqueous side of the air-sea interface for both turbulent and radiation heat loss to the atmosphere (Minnett et al. (2011)). Molecular
conduction also explains the establishment of the thermal skin layer’s strong temperature gradient because it is a less efficient method of heat transfer as compared to turbulence, which occurs on the oceanic mixing layer beneath the thermal skin layer, or convection, which occurs in the atmospheric boundary layer. The EM skin layer exists due to EM properties of water which controls the absorption and emission of IR radiation. This emission comes from depths of less than 1 mm and the radiation measured by IR radiometers on ships and satellites has its origin in this layer. The ship-board spectra-radiometers, e.g. the Marine Atmospheric Emitted Radiance Interferometers (M-AERIs), have a footprint of \( \sim 1 \text{ m}^2 \) depending on the distance of the instrument from the ocean’s surface, therefore it is important to note that the measured IR spectra are radiances averaged over many sea surface renewal events. Radiometric measurements of the skin SST from ships have been performed extensively over the past few decades in a wide range of conditions, particularly in studies with wind speed and the diurnal cycle, both of which have a significant effect on the gradient of the thermal skin layer (eg. McAlister and McLeish (1969); Schluessel et al. (1990); Minnett et al. (2001); Donlon et al. (2002); Minnett (2003)). In-situ measurements made in the past several decades have also confirmed the presence of a cool-skin layer (e.g. Woodcock and Stommel (1947); Katsaros et al. (1977); Donlon et al. (2002); Ward et al. (2004); Ward (2006)) and have shown it to be a non-linear thermal structure which, and quoting from Spangenberg and Rowland (1961), ‘varies approximately exponentially with depth’. Fairall et al. (1996a) and Jessup et al. (1997) have also shown that the thermal skin layer is only disrupted momentarily by wave breaking or during high winds with speeds > 10 \text{ m/s}, after which the thermal skin layer returns to its former condition very quickly in a matter of seconds. This means that the thermal skin layer is almost
always present and should always be considered during the analysis of any processes involving SSTs.

SST observations have shown that ocean heat content has been increasing notably over recent decades (Lyman et al., 2010). The question is: "how does an increase in greenhouse gases, such as carbon dioxide and methane, cause an increase in the ocean temperature"? In a balanced Earth’s radiative heat budget system over the ocean, the incoming shortwave (SW) and incoming longwave (LW) radiation equals the outgoing LW radiation, latent heat and sensible heat fluxes. The EM skin layer absorbs and re-emits IR radiation while the heat provided by molecular conduction down the temperature gradient in the thermal skin layer provides energy to sustain the latent and sensible heat losses at the interface and makes up the difference between the absorbed and emitted IR radiation within the EM skin layer. The SW radiation penetrates to deeper depths and the greater part (> 99%) is absorbed in layers beneath the skin layer. An increase in greenhouse gases would cause an increase in incoming LW radiation which gets absorbed in the EM skin layer, thus increasing the temperature of the thermal skin layer and resulting in a surplus of energy. The surplus of energy could now be fed to the outgoing LW, latent and sensible heat fluxes at the air-sea interface which was previously supplied by the energy from absorbed SW radiation beneath the thermal skin layer. The SW radiation would therefore be trapped beneath the thermal skin layer resulting in a temperature rise in the bulk of the ocean. If the temperature in the bulk of the ocean increases while the temperature at the surface varies slightly, the only way that this temperature difference can be supported is by changes in the gradient of the thermal skin layer. Therefore, observing gradient changes in the thermal
skin layer may potentially help predict the amount of heat trapped in the bulk of the ocean due to an increase in greenhouse gases.

Despite its importance, the thermal skin layer is not well-understood and there have been few attempts to retrieve the thermal skin layer vertical profile due to the complexity of the influence of variables such as wind-speed and surface tension effects on this very thin structure. Most attempts made in measurements of the thermal skin layer profile have been conducted using mechanically invasive probes which pose a high-risk in changing the thermal skin layer gradient since the fine-wire measurements would directly heat or physically disrupt the skin SST (e.g. Katsaros et al. (1977); Ward et al. (2004)). As such, passive remote sensing is ideal since these sources of errors would be eliminated. McKeown et al. (1995) and Hanafin (2002) demonstrated the use of radiometers in the IR and near-IR region in laboratory experiments to obtain the thermal skin layer gradient but with an assumption that the temperature gradient is linear. The objective here is to demonstrate the retrieval of the thermal skin layer’s non-linear profile using ship-board data taken by the Marine-Atmospheric Emitted Radiance Interferometer (M-AERI) and to understand the curvature of the thermal skin layer where the heat flux flows from the ocean to the atmosphere. The remote-sensing group in the Rosenstiel School of Marine and Atmospheric Science (RSMAS), University of Miami, is one of the very few research groups with the ability to perform ship-board measurements of skin SST. The M-AERI’s have been deployed in a large number of cruises over the past 10 years and are well suited for the problem to be addressed here given their high accuracy of the spectrally-resolved measurements of the thermal emission from the thermal skin layer.
Chapter 2

Data

The data used in this study consists of experimental synthetic datasets designed to test and evaluate the retrieval technique adopted and also taken from a 2006 field campaign: the African Monsoon Multidisciplinary Analysis (AMMA), to demonstrate the technique's robustness. The first section describes the instrumentation and the conditions in which the cruise data were taken. This is followed by an outline of the quality controls applied to the field data. The last section describes the generation of synthetic data together with a review of the theoretical background on the different formulas for the gradient of the thermal skin layer.
2.1 Field Program

2.1.1 Instrumentation: Marine-Atmospheric Emitted Radiance Interferometer (M-AERI)

The M-AERI is a sea-going, passive, well-calibrated, Fourier Transform Infrared (FTIR) interferometer. It was developed from the Atmospheric Emitted Radiance Interferometer (AERI) at the Space Science and Engineering Center, University of Wisconsin-Madison which was originally built for the Department of Energy’s Atmospheric Radiation Measurement Program. The M-AERI measures radiances (units: $W m^{-2} S r^{-1} cm^{-1}$) emitted across the wavenumber range 500-3000 $cm^{-1}$ ($3-20 \mu m$) with an effective spectral resolution of 0.5 $cm^{-1}$ which allows for gaseous absorption and emission lines in the atmosphere to be resolved. Minnett et al. (2001) describe the details of its operations, accuracy and applications and a brief introduction will be given here.

Figure 2.1 shows a M-AERI on the National Oceanic and Atmospheric Administration (NOAA) Research Vessel (R/V) Ronald H. Brown (RHB), as seen from the deck below. Shown also in Figure 2.2 is the exposed D-shaped compartment on the right-hand side of the M-AERI and contains a scanning mirror, two blackbodies (BB) for calibration and a mirror motor. The left-hand side, known as the main compartment, contains a sealed FTIR unit, an optics chamber, IR detectors, Stirling cycle cooler and other electronics. Two infrared detectors, made from Indium Antimonide (InSb) for the higher wavenumber range (1800-3000 $cm^{-1}$) and Mercury Cadmium Telluride (HgCdTe) for the lower wavenumber range (520-1800 $cm^{-1}$), are cooled to near ~78 K by the Stirling cycle mechanical cooler in order to reduce the noise equivalent temperature differ-
Figure 2.1: M-AERI deployment on the NOAA research vessel Ronald H. Brown. The instrument is on the forward O2 deck at the starboard railing and the field of view intersects the sea surface ahead of the bow wave. (Minnett et al., 2001).

ene (NE\(\Delta T\)) to levels well below 0.1 K. Accurate real-time calibration is also achieved by the two internal BB cavities which are fixed to a structure which supports the scan mirror motor, with their axes at 60° and 120° with respect to the vertical. The upper one is heated to 60°C while the lower one is at ambient air temperature.

The M-AERI operates through a sequence of pauses in the rotation of the scanning mirror. The mirror is located at the intersection of the long axes of the two BBs (Figure 2.2) and is tilted 45° to its axis of rotation which is perpendicular to the surface of the main compartment. The mirror therefore directs the incoming radiation towards the main compartment and into the field of view (FOV) of the FTIR unit.
Figure 2.2 shows a schematic of the M-AERI’s viewing geometry. Each sequence of scene view consists firstly of the upwelling radiance from the sea surface and the downwelling atmospheric radiances measured at complementary angles with typical at-sea deployment measured incidence angles, $\theta_i$, of $55^\circ$, followed by a zenith measurement of the downwelling radiation. The calibration sequence which consists of measurements of the emission from the two BBs shown in Figure 2.2, brackets each set of scene views. This calibration sequence is tested using a 3-body calibration technique in which a third BB is placed in the FOV of the M-AERI and comparisons between the measured brightness temperatures (BT) and BB temperatures are made. Tests demonstrated that
measurement errors are within 0.02 K (Figure 2.4) with the two BB calibration scheme producing BT with errors of <0.03 K in the 800-1200 cm\(^{-1}\) range at 20-30°C. These tests are performed in accordance to sensors calibrated to the National Institute of Science and Technology (NIST) standards (Figure 2.5) (Minnett et al., 2001). The signal-to-noise (SNR) ratios range from 175-800 for the long-wave (HgCdTe) detector and 20-467 for the short-wave (InSb) detector for the target noise equivalent radiance differences (NE\(\Delta L\)). When averaged over 45 independent interferograms, which is routinely done in at-sea operations, the SNR increases to 1135-5400 and 135-3135 for the long-wave and short-wave detectors respectively. Typical skin SST measurements are derived at a wavelength of 7.7\(\mu m\) which corresponds to radiance values of \(\sim 55\) mW\(m^{-2}\)sr\(^{-1}\)cm\(^{-1}\) and a SNR of \(\sim 270\) for a single interferogram or \(\sim 1800\) for a 45-s average. The entire full 3-scene sequence with calibration takes 8-12 minutes. Data
quality may be compromised from possible water droplets in the air such as fog, rain and sea-spray which might cause slight corrosion of the scene mirror but is generally not affected by other weather conditions such as high wind speeds. A rain sensor halts the routine sampling when rain or spray are detected. The operation is fully automatic once the initial set-up is complete. For long periods of bad weather, the instrument is protected under a tarpaulin.

Figure 2.4: Temperature difference measured by the M-AERI and a calibrated blackbody placed in its FOV. (Minnett et al., 2001)
Figure 2.5: Comparison between the temperature measured by the M-AERI and that of a NIST blackbody at 60°C (upper panel), 30°C (middle panel) and 20°C (lower panel). (Minnett et al., 2001)
Figure 2.6: Sample of M-AERI radiance data and its equivalent brightness temperature during night-time and cloud-free conditions. Blue line - upwelling radiance measurement at 55°; Red line - downwelling radiance measurement at 55°; Black line - downwelling radiance measurement at zenith.

The top panel of Figure 2.6 shows a sample radiance spectrum from the M-AERI taken during night-time and cloud-free conditions across the full wavenumber range of 500-3000 cm$^{-1}$. The bottom panel shows the radiances converted into spectral BT using Planck’s function. The blue lines indicate the upwelling radiance from the sea surface and exhibit a typical smooth Planckian shape with the exception of random spikes observed at frequencies where the signal is masked by thermal noise (e.g. 1500-1700 cm$^{-1}$) because the atmosphere is not sufficiently transmissive for the calibration.
to function well. From the bottom panel, the 'drop' in the atmospheric BT values at frequencies of 700-1300 cm$^{-1}$ and 2000-2900 cm$^{-1}$ indicates the presence of atmospheric windows. This means that the atmosphere is transmissive in these window regions and allows the M-AERI to observe radiances emitted from layers higher up in the atmosphere. Outside of the atmospheric transmission window regions, the atmosphere is less transmissive and the measured temperature from the M-AERI is warmer because it is sensing radiation emitted from gases in the lower parts of the atmosphere.

With reference to Figure 2.3, the observed upwelling radiance, $R_{\text{sea}}$, measured by the M-AERI while viewing the sea surface consists of the spectral radiation emitted by the sea surface, the incident radiation, $R_{\text{sky}}$, reflected at the sea surface and the component of atmospheric emission from the layer below the level of the instrument at height $h$, $R_{h}(v, \theta)$, which includes both direct and reflected emission from the sea surface attenuated by the atmosphere between the surface and height $h$. This is expressed in Equation 2.1 and described by Minnett et al. (2001) and Hanafin (2002).

$$R_{\text{sea}}(v, \theta) = \epsilon(v, \theta)B(v, T_{\text{skin}}) + (1 - \epsilon(v, \theta))R_{\text{sky}}(v, \theta) + R_{h}(v, \theta)$$

(2.1)

where $v$ is the wavenumber, $R_{\text{sea}}(v, \theta)$ is the calibrated radiance measurements made at nadir angle, $\theta$ and $v$; $B(v, T_{\text{skin}})$ is the sea surface spectral radiance emission at $v$ and temperature, $T_{\text{skin}}$; $R_{\text{sky}}$ is the downwelling atmospheric radiance emission at nadir angle, $\theta$, and $v$; $\epsilon(v, \theta)$ is the sea surface emissivity at $v$ and emission angle $\theta$. 
Since the M-AERI is mounted on a ship at a height of a few meters, $R_h(v, \theta)$ is very small and will be neglected in the analysis used in this research. Rewriting equation 2.1 without $R_h(v, \theta)$:

$$R_{sea}(v, \theta) = \varepsilon(v, \theta)B(v, T_{skin}) + (1 - \varepsilon(v, \theta))R_{sky}(v, \theta)$$  \hspace{1cm} (2.2)

Solving for the skin sea surface temperature, $T_{skin}$ gives:

$$T_{skin} = B^{-1}\{(R_{sea}(v, \theta) - [1 - \varepsilon(v, \theta)]R_{sky}(v, \theta))/\varepsilon(v, \theta)\}$$  \hspace{1cm} (2.3)

where $B^{-1}$ is the inverse Planck function. Equation 2.3 is used to perform the atmospheric correction and to retrieve the skin SST value from M-AERI measurements of spectral radiances, $R_{water}$ and $R_{sky}$.

### 2.1.2 African Monsoon Multidisciplinary Analysis (AMMA) 2006 cruise

The African Monsoon Multidisciplinary Analysis AMMA 2006 cruise on the R/V RHB took place in the tropical Atlantic Ocean from May 28 to July 14, 2006 and M-AERI data collected during this cruise will be analyzed for this research effort. AMMA was a coordinated international project conducted to improve knowledge and understanding of the West African Monsoon (WAM), its variability and impacts. The objective of deploying the M-AERI was to validate SST retrievals from radiometers on National Aeronautics and Space Administration (NASA) satellites in the tropical Atlantic, and to
study and characterize the Saharan air layer (SAL). There were 2 legs: Leg 1 was from May 28 to June 17 with the RHB leaving San Juan, Puerto Rico, heading south-east with the majority of the leg spent off West Africa. Leg 2 was from June 22 to July 14, leaving Recife, Brazil and steamed north to Charleston, SC. Cruise tracks with SST measurements made by the M-AERI are shown in Figure 2.7.

The M-AERI was installed on the starboard side of the O2 deck of the R/V RHB, with a pointing angle of 55° to nadir. Retrievals of the skin layer temperature profiles from M-AERI spectra measurements were done beginning on May 27 and ending on July 14, 2006. The gap from May 27 - June 22 corresponds to the port call in Recife, Brazil, while the other larger gaps in M-AERI data were due to instrument failure or periods of bad weather. The M-AERI was repaired and data collection was restored on July 29. The SST ranges from 295 K to 305 K.

This cruise was chosen because of the availability of ceilometer data which enables the presence of clouds to be detected and relatively low wind speeds with a mean of 7.8 m/s. A summary of the statistics of meteorological variables are: air temperatures ranged from 295 K to 302 K, air pressure readings were in the interval of 1010 hPa to 1030 hPa, relative humidity ranged from 50 to 80 % and wind speeds occurred at 0 m/s to 20 m/s. For the purpose of this analysis, only night-time data (20:00 - 08:00 h local time) were processed to avoid possible contamination of the measurements by reflected and scattered solar radiation. Data taken in the presence of clouds were excluded from the analysis as discussed in Section 2.2.
Figure 2.7: AMMA 2006 cruise tracks with SST measurements made by the M-AERI. Top panel shows SST measurements taken during Leg 1 while the bottom panel shows SST measurements taken during Leg 2. Dates show the position of the ship at the start of each UTC day; gaps are caused by rain or heavy sand when useful data cannot be taken.
2.2 Quality control of field data

Figure 2.8 shows an example of a dataset obtained from the M-AERI in the atmospheric windows during cloud-free, night-time conditions with the atmospheric corrected BT spectrum plotted as the blue line. Spectra which show the presence of clouds were removed as emission from clouds mask the atmospheric emission lines. The presence of atmospheric emission lines is important in order for the atmospheric corrections to be accurately performed since it shows contrast between the sea measurement (upwelling radiance spectrum, $R_{\text{water}}$) and sky measurement (downwelling radiance spectrum, $R_{\text{sky}}$). This contrast is required for the derivation of spectral emissivity using a variance minimizing technique described by Hanafin (2002) and is described in Section 3.1. Without this contrast, an invalid emissivity value would be derived.

The presence of passing clouds overhead would also introduce temporal and spatial heterogeneity because the M-AERI operates by the use of a scanning mirror which measures the sea and sky radiances consecutively and not simultaneously. Thus, changing cloud conditions may introduce uncertainty in the reflected sky emission correction. Clouds pose an additional problem in rough sea surfaces as it may introduce additional error due to facets of tilted sea surfaces in the M-AERI’s field of view causing specular reflection of the sky radiance away from the simple geometric path shown in Figure 2.3.
Figure 2.8: Sample Radiance Spectrum (upper panels) and their spectral brightness temperatures (lower panels) obtained from the M-AERI during night-time and cloud-free conditions. Red line shows the upwelling radiance or BT spectrum retrieved. Black line shows the downwelling radiance spectrum retrieved. Blue line shows the corrected upwelling BT spectrum.
2.3 Synthetic datasets

The primary goal of generating synthetic datasets is to test the robustness of the thermal skin layer’s retrieval algorithm developed. The truncated singular value decomposition (TSVD), to be described in Section 3.3, requires a good first guess profile which must be a close representation of the expected retrieved profile. Therefore, it is important to understand what are the possible forms of the thermal skin layer temperature profile in order to have a good gauge and a form of verification when the retrieval is attempted. There have been a number of theoretical approaches in understanding the thermal skin layer, namely in the study of surface fluxes and by dimensional analysis (Saunders, 1967). The first section of this chapter describes the model adopted to represent the thermal skin layer, followed by a description of the set of sample synthetic datasets to be used in our retrieval runs in order to understand and validate the feasibility and robustness of the model used in the retrieval.

2.3.1 Theoretical molecular thermal skin sea surface temperature profile

A bulk surface flux model was described by Liu and Businger (1975). They made partial use of the surface renewal theory to derive temperature profiles representative of the thermal skin layer. Their results will be adopted here. Starting with the heat diffusion equation which governs the molecular heat transfer in the thermal skin layer:

\[
\frac{\partial T}{\partial t} = \kappa \frac{\partial^2 T}{\partial z^2}
\]  
(2.4)
Liu and Businger (1975) took a scaling depth, $\delta_c$, to be that of a purely conductive heat flux, $Q_0$, such that $\delta_c = \kappa \frac{T_s - T_b}{\bar{Q}_0}$, where $\kappa$ is the thermal conductivity of water and $\bar{Q}_0$ represents the purely conductive heat flux averaged over time or space. Thus, the solution is approximate for the mean thermal skin layer averaged over many surface renewal events. They solved Equation 2.4 for $T(z,t)$ for 3 different cases and found the temperature profile to be of the form of a complementary error function ($\text{erfc}$) for the cases of free convection with 2 different boundary conditions, while an exponential function for the case of forced convection. The derived cases are given below:

(a) Forced convection with a constant sub-skin temperature, $T_b$, and constant skin temperature, $T_s$, boundary condition gave a temperature profile:

$$\frac{T - T_b}{T_s - T_b} = e^{-z/\delta_c}$$  \hspace{1cm} (2.5)

Khundzhua and Andreev (1974) measured temperature profiles in sublayers of laminar flow near the air-sea interface 30 miles off-shore in the Black Sea, and showed a similar exponential function as Equation 2.5.

(b) Free convection with a boundary condition of a constant temperature difference between the sub-skin temperature, $T_b$ and the skin temperature, $T_s$, resulted in a temperature profile of:

$$\frac{T - T_b}{T_s - T_b} = 4i^2\text{erf}c\left(\frac{\sqrt{\pi}z}{4\delta_c}\right)$$  \hspace{1cm} (2.6)

where $4i^2\text{erf}c(x) = (1 + 2x^2)\text{erf}c(x) - \frac{2xe^{-x^2}}{\sqrt{\pi}}$. 
(c) Free convection with a constant heat flux boundary condition gave a temperature profile with the form:

\[
\frac{T - T_b}{T_s - T_b} = \pi^{0.5} 6i^3 \text{erf} c\left(\frac{2z}{3\pi^{0.5} \delta_c}\right)
\]

(2.7)

where \(6i^3 \text{erf} c(x) = \frac{(1+x^2)e^{-x^2}}{\sqrt{x}} - (1.5 + x^2)\text{erf} c(x)\)

Equation 2.7 was adopted here as the first-guess model because for most of the time, we are dealing with free convection in the open ocean. Furthermore, since attempts are being made to retrieve the temperature profile of the thermal skin layer, it is preferable not to have any assumptions made for the temperature values. Thus, the case of a constant heat flux boundary condition was chosen.

2.3.2 Synthetic dataset parameters

A sample profile, \(T_{\text{original}}(z)\) was generated from Equation 2.7 using the following parameters: \(T_s = 301 K, T_b = 301.3 K, Q_0 = 50 W/m^2\) and was representative of the actual temperature profile of the skin layer. In addition, 3 other profiles were generated and used as first-guess profiles in attempts to retrieve \(T_{\text{original}}(z)\):
Case 1: An erfc curve (Equation 2.5), with the same $T_s$ and $T_b$ values as $T_{\text{original}}(z)$ but with a different curvature obtained by varying $Q = 20 \text{ W/m}^2$.

Case 2: A piece-wise linear profile with the same $T_s$ and $T_b$ values as $T_{\text{original}}(z)$ but with a discontinuity at in the vertical gradient $z = -0.02 \text{ cm}$.

Case 3a: An erfc curve (Equation 2.5), fitted to the BTs obtained from the spectral radiance values which are calculated by substituting $T_{\text{original}}(z)$ into Equation 3.3.

Case 3b: As 3a but the first guess $T_b$ value is incremented by 0.7 K.

Figure 2.9 shows the generated $T_{\text{original}}(z)$ and $T_{fg}(z)$ cases. The profiles are extended to a depth of 0.1 cm with intervals of 0.00001 cm so as to perform the integration of Equation 3.3 by use of a trapezoidal rule. For the TSVD method a 100 point-Gauss Legendre quadrature rule was used. The depth was extended to 0.04 cm when the Gauss Lengendre rule was used in evaluating the integral. Details on the integral equation to be solved are described in Section 3.2.2 and the application of the TSVD method are described in Section 3.3.
Figure 2.9: Plots of Synthetic datasets generated of the assumed original profile, $T_{\text{original}}(z)$, and first-guess profiles from Cases 1, 2 and 3a. $T_{fg}(z)$. Subscript fg represents the first-guess.
This chapter outlines the principles and methods used behind the techniques and considerations made in our analysis. The technique used to derive the sea surface spectral emissivity is first described, followed by the theoretical background and explanation on the fundamentals as to how the thermal skin layer profile is obtained from the M-AERI's spectral radiances. The last section discusses a classical regularization method known as the truncated singular value decomposition which is used in the retrieval of the thermal skin layer.

3.1 Determining sea surface spectral emissivity

3.1.1 The piecewise linear variance minimization technique (VarMinT)

As shown in Equation 2.2 the emissivity value is an important parameter in calculating the atmospheric correction before attempts to solve the inverse problem of Equation 3.3
can be made. In order to derive the spectral emissivity values, a piecewise linear variance minimizing technique is used whose robustness was analyzed by Hanafin (2002). This technique, termed VarMinT, selects a small wavenumber range ($< 10 \text{ cm}^{-1}$) and calculates the variance of the BT (Equation 2.3) for a set of prescribed emissivity values, $\varepsilon$. The emissivity value corresponding to the minimized BT variance is taken to be the value across this wavenumber segment. The assumptions for the VarMinT are that the sky radiance, $R_{sky}$, is not correlated with the sea surface emissivity spectrum and the sea surface emissivity spectrum is a smooth function with wavenumber. Rearranging Equation 2.2 gives:

$$\varepsilon = \frac{R_{water} - R_{sky}}{B(v, T_{skin}) - R_{sky}}$$ (3.1)

To further minimize sources of error arising from uncertainties in the refractive index data for seawater and measurement limitations, such as the presence of a time lag between the sequential measurement of the downwelling, $R_{water}$ and upwelling, $R_{sky}$ radiance resulting in different spectral signatures in the emissivity and upwelling radiances, a piecewise linear approach is adopted. This approach calculates the emissivity of the measurements using 3 different wavenumber segments ($5 \text{ cm}^{-1}$, $10 \text{ cm}^{-1}$, $15 \text{ cm}^{-1}$) and averages them into $10 \text{ cm}^{-1}$ ranges such that at least 4 estimates occur in each $10 \text{ cm}^{-1}$ average. The spectrally binned average is subsequently passed through a digital box-car low-pass filter to produce a smooth spectral emissivity. Figure 3.1 shows the emissivity values from a spectra which was obtained from averaging 5 radiance spectra from the AMMA06 cruise dataset. Only the 2 wavenumber ranges identified in Section 2.2 are shown.
Also plotted in Figure 3.1 are the emissivity values calculated by Filipiak (2008) at a 55° view angle, 0 m/s wind speed and at a water temperature of 300 K with a salinity of 35 psu. The results obtained from the VarMinT method agrees well with Filipiak's data but with some slight discrepancies which may be due to differences in the dataset’s environmental conditions (e.g. wind speed, temperature, salinity) compared to those of Filipiak. Furthermore, Filipiak emissivity values are derived from relative reflectances of water whereby effort was made in laboratories to ensure that the water and all surfaces are as clean as possible. Real seawater conditions, on the other hand, most likely include surfactants and slight impurities which would cause small variations in the emissivity value. The differences in Figure 3.1 are less than 0.005 and are not of major concern in the calculation of the BT’s being retrieved.

### 3.1.2 Emissivity sensitivity tests

To ensure that the emissivity values derived from the piecewise linear VarMinT are suitable for our study of the thermal skin layer, two sensitivity analyses with respect to emissivity at 2 wavenumber regions were attempted. The selection of these 2 wavenumber ranges are described in Section 3.2.1. The first test involved varying the emissivity at increments of 0.005, 0.001, 0.0005 and 0.0001 for the VarMinT. This is to ensure that the results derived using an emissivity interval of 0.0005 for the VarMinT algorithm are robust. Figure 3.2 shows the resultant spectral emissivity values derived for the 4 increments chosen and Figure 3.3 corresponds to the difference between the emissivity values calculated at increments 0.005, 0.001 and 0.0005 with the spectral emissivity derived at an incrementation of 0.0001.
It is shown that the difference is insignificant when increments of 0.0005 and 0.001 are used when comparisons are made with the spectral emissivity values derived using an increment of 0.0001. There is a small significant change in the emissivity derived using an increment of 0.005. In general, at the wavenumber regimes chosen, the change in emissivity values are $< 10^{-3}$ which means our derived emissivity values are at an accuracy of $< 0.1\%$ for an incrementation choice of 0.0005 and 0.001. This indicates that an accuracy of 0.001 in the emissivity derived using the VarMinT algorithm can be
Figure 3.2: Spectral emissivity values derived for 4 different emissivity incrementation values in the VarMinT using a sample AMMA 2006 cruise measurement. Black line: increment of 0.0001; red line: increment of 0.0005; blue line: increment of 0.001; green line: increment of 0.005.

achieved giving us confidence in the sea surface BT retrieved from the M-AERI measurements, and that the deviation from Fillipak’s emissivity values seen in Figure 3.1 are not caused by algorithm artifacts.

The second sensitivity test relates the changes in emissivity to changes in BT. For this test, the spectral emissivity values derived with an increment of 0.0005 in Figure 3.2 were decremented by a factor of 0.01 and a plot of the gradient, i.e. $S_e = \frac{\Delta(BT)}{\Delta e}$ as a function of wavenumber is shown in Figure 3.4.
Figure 3.3: Difference of spectral emissivity values derived for increments of 0.005, 0.001 and 0.0005 and comparing it with values derived with an incrementation of 0.0001 in the VarMinT using a sample AMMA 2006 cruise measurement. Spectral emissivity derived using an incrementation of: Red line: 0.0005; blue line - 0.001; green line - 0.005.

A blue dotted reference line of $S_e = 20$ is also drawn. This line means that a 0.01 change in emissivity would result in a 0.2 K change in temperature. Above this line, small changes in emissivity would results in larger BT variations, i.e. BT is more dependent on the emissivity value, and vice versa. From Planck’s law, the percentage change in radiance to a percentage change in BT, $S_{BT} = \frac{\Delta B(v,T)/B(v,T)}{\Delta BT/BT}$, increases with increasing wavenumber in the IR region. Therefore, changes in emissivity affects the changes in radiances and we expect $S_e$ to increase with increasing wavenumber. This is shown particularly in the wavenumber range of 800-1000 cm$^{-1}$ as there are is a rapid radiance drop ($120-50$ mW m$^{-2}$Sr$^{-1}$ cm$^{-1}$). However, $S_e$ does not continue to increase steadily
Figure 3.4: Plot of sensitivity of BT to emissivity values and upwelling sky radiance against wavenumber because of a plateau in radiances from 1000-1200 \( cm^{-1} \) at \( \sim 50 \text{ mW m}^{-2}\text{Sr}^{-1}\text{cm}^{-1} \) and 2640-2800 \( cm^{-1} \) at \( \sim 0.15 \text{ mW m}^{-2}\text{Sr}^{-1}\text{cm}^{-1} \). The main reason for the variability of the \( S_e \) values of these wavenumbers are due to lower emissivity values \( (\epsilon \sim 0.95) \) obtained from 2640-2800 \( cm^{-1} \) compared to the 1000-1200 \( cm^{-1} \) range \( (\epsilon \sim 0.97) \). This implies that a constant offset in the emissivity would have a larger effect on the BT for wavenumbers with higher emissivity values (Equation 3.1). Thus, the magnitude of the derived emissivity is the dominating factor for the variability in \( S_e \) resulting in a lower \( S_e \) for the range 2640-2800 \( cm^{-1} \) since \( \epsilon \) is lower.
Plotted with Figure 3.4 is the downwelling sky radiance. Note that regions in which the downwelling sky radiance ‘peaks’, the gradient experiences a ‘trough’, because when the downwelling sky radiances peaks, the contrast between the upwelling sea radiance and downwelling sky radiance measurement is small resulting in a worsened estimate of the emissivity, (the denominator in Equation 3.1 approaches zero). The ‘peaks’ occur due to changes in atmospheric transmissivity traversing down the spectrum (Figure 2.6). Figure 3.5 shows a sample BT with depth profile before and after the emissivity correction is performed. The larger oscillations seen at deeper depths can therefore be explained as the measured downwelling sky radiance spectrum being more variable at higher wavenumbers imply there is more variability in the contrast required for the VarMinT to produce the emissivity value. Thus, the oscillations seen are deemed unphysical.

3.2 Profiling the thermal skin layer

3.2.1 Theoretical background

The physics behind skin depth measurements of seawater using infrared (IR) radiation involves knowledge of the penetration and emission depth in the IR part of the electromagnetic (EM) spectrum. Beer-Lambert’s law explains that the incident radiation with intensity, $I_0$, is attenuated to $1/e$ of its original intensity after it has travelled through a pathlength of $D_p = 1/\alpha$, also known as the penetration depth:

$$I(z) = I_0 e^{-\alpha z} \quad (3.2)$$
Figure 3.5: Plot of brightness temperature with depth. Measurement values obtained from a sample AMMA 2006 cruise radiance spectrum.

where $\alpha$ is the absorption coefficient of the medium and can be found from the wavenumber, $\nu$, of the incident radiation and the corresponding imaginary component of the refractive index of the medium, $k$, ($\alpha = 4\pi k \nu$). Values of $k$ for water are obtained from Bertie and Lan (1996).

In the IR region, a large fraction of the EM radiation penetrates the water surface to a fraction of a millimeter in depth, which means that the majority of the radiation sensed by radiometers operating in the IR regime is emitted from these shallow depths. There are slight variations of the penetration depth at different frequencies due to small changes in $\alpha$ at different wavenumbers. This relationship is shown in Figure 3.6. The graph shows that radiation emitted at wavenumbers of around 2400-2600 cm$^{-1}$ comes
from a thicker layer of the water column than at lower frequencies in which the absorption coefficient is greater. By Kirchoff’s law of thermal radiation, the emissivity of a body or surface equals its absorptivity at thermodynamic equilibrium. Thus, the penetration depth, in which the majority of radiation is absorbed, would equal the emission depth. The approach here is to use the penetration depth to measure the temperature profile through the thermal skin layer by directly mapping the brightness temperature spectrum retrieved from the M-AERI to the penetration depth with reference to their corresponding wavenumber (Hanafin, 2002; McKeown et al., 1995). This direct mapping method of retrieving the thermal skin layer profile is a good first approximation if one is interested in obtaining a rough estimate of the profile of the skin layer.

The 2400-3000 cm$^{-1}$ range was identified by McKeown et al. (1995) as appropriate and effective sounding channels for retrieving the thermal skin SST profiles. Hanafin (2002) identified the frequency ranges: 800-1200 cm$^{-1}$ and 2400-2800 cm$^{-1}$ using experimental studies made by the M-AERI. The requirements identified for these window ranges are that there is minimal atmospheric absorption such that it is deemed negligible, the reflectance of water is weakly dependent on the temperature and salt content and there is a good depth range. The ranges used in this study are 800-1200 cm$^{-1}$ and 2640-2800 cm$^{-1}$ and are further limited to avoid duplicate BT values at the same $D_p$ since $D_p$ at 2400-2640 cm$^{-1}$ coincides with 2640-2800 cm$^{-1}$ and would cause the inverse problem to be over-constrained (Section 3.2.2).
Figure 3.6: Plot of penetration depth, $D_p$, vs wavenumber $\nu$. Imaginary component of the refractive index of water, $k$ values to calculate $D_p = \frac{1}{4\pi kv}$ are obtained from Bertie and Lan (1996).

### 3.2.2 The non-linear inverse problem

A down-looking interferometer such as the M-AERI senses radiation coming from 2 origins: the sea surface and the intervening atmosphere. Equation 2.2 is representative of the radiance being emitted by the sea surface without the components of reflected sky radiance and the intervening atmosphere. To retrieve the non-linearity of the thermal skin layer, it is necessary to assess the total amount of radiation being emitted from the sea surface due to each underlying water layer from the sea surface. By dividing the ocean into infinitesimal layers each with a temperature $T(z)$, where $z$ is the depth of the layer, the radiation being emitted into the atmosphere from the sea surface from each layer can be simply thought of as the radiative transfer between 2 parallel plates.
(one being the surface of the ocean, the other is the layer at depth \( z \)), attenuated by
the intervening layer. The attenuation factor is defined by Beer-Lambert's law (Equa-
tion 3.2) and the total amount of radiation emitted from the sea surface would be the
summation of each attenuated radiance:

\[
I_m(v) = -\int_0^\infty B(v, T(z)) \cdot \frac{d(e^{-az})}{dz} \, dz
\]

(3.3)

where \( I_m(v) \) is the measured radiance at wavenumber \( v \) in cm\(^{-1} \), \( B(v, T(z)) \) is
Planck's function with \( T(z) \) being the vertical temperature profile to be found, and
\( \frac{d(e^{-az})}{dz} \) is the weighting function given by Beer’s law. The negative sign refers to a
higher attenuation factor for layers at deeper levels since we define \( z = 0 \) at the surface
of the ocean and \( z = -\infty \) at depth.

Equations 3.3 and 2.2 can therefore be used to retrieve the vertical temperature
profile, \( T(z) \), given the radiance spectra measured by the M-AERI. The issue here is
that Equation 3.3 is a non-linear Fredholm equation of the first kind and is known
to be ill-conditioned (Eyre, 1987; Rodgers, 2004) which means that the errors in the
measurements are amplified resulting in a possibly meaningless solution even if the
least squares fit solution agrees with the measurements. The numerical approximation
of Equation 3.3 can be written in the form:

\[
y = Ax
\]

(3.4)

where \( y \) represents the set of measured radiance values, \( x \) is the set of temperature
values and matrix \( A \) defines the conversion from the temperature to radiances values.
The solution, $x$, is unique only if the following 2 conditions are both satisfied: $y$ is in the range of $A$ and the kernel of $A$ is a null space. This would therefore allow the inverse of matrix $A$ to exist and a unique solution to occur. In reality, $y$ is usually measured data and include uncertainties leading to $y \approx Ax$. $y$ and $x$ must therefore occur in finite-dimensional spaces in order for $A^{-1}$ to be continuous and a solution be found, else small errors in $y$ would result in amplification of errors in $x$. We can derive a sense of the ill-conditioning of the problem by examining the condition number of matrix $A$, $\kappa(A) = ||A^{-1}|| \cdot ||A||$, also defined as the maximum ratio of the relative error in $\frac{x}{y}$. An ideal condition number is 1, meaning that convergence may occur in the solution and be obtained with some arbitrary precision. A high condition number implies an inaccurate solution may be obtained since a small error in $y$ may result in amplification of errors in $x$. In this case, $\kappa(A)$ is large, of an order of $\sim 10^{21}$ which means that the matrix is highly ill-conditioned and an inverse of the problem would be largely contaminated by errors.

There are a variety of techniques called regularization methods to solve these types of ill-posed problems. The main idea of regularization methods is to constrain the solution by introducing an additional criterion such that optimal convergence towards the true solution would occur. The regularization technique adopted in this study is called the Truncated Singular Value Decomposition (TSVD) and is further described in Section 3.3.
3.3 **Truncated singular value decomposition (TSVD)**

The TSVD method is a well-known regularization method for solving ill-posed linear least squares problems and is described in detail in Hansen (1990). A brief discussion of the TSVD would be explained in the first section followed by the application of the TSVD method to the inverse problem (Equation 3.3).

### 3.3.1 Theory: truncated singular value decomposition

For the linear ill-conditioned problem of Equation 3.4, performing a singular value decomposition on matrix $A$ decomposes $A$ into three matrices $U$, $S$ and $V$:

$$A = USV^T$$  \hspace{1cm} (3.5)

where the non-singular matrix, $U \in \mathbb{R}^{m \times m}$ and non-singular matrix, $V \in \mathbb{R}^{n \times n}$ are orthogonal and the matrix, $S \in \mathbb{R}^{m \times n}$ is a diagonal with elements $\sigma_i$ which are the singular values of $A$. The elements of $S$ are ordered such that:

$$\sigma_1 \geq \sigma_2 \geq ... \geq \sigma_r > 0,$$

where $r = \text{rank}(A)$

The concept behind the TSVD is to impose an additional requirement on the solution such that a well-conditioned number for the matrix $A$ is obtained. This would damp out undesired contributions from errors in the measurement vector, $y$. The TSVD method achieves this by neglecting components of the solution corresponding to the smallest singular values because these contributions are the cause of the magnification of the errors in the solution. Therefore, by removing these components and defining $A$ to be a rank-$p$ matrix, we get:
\[ A_p \equiv US_p V^T, \quad S_p = \text{diag}(\sigma_1, ..., \sigma_p, 0, ..., 0) \in \mathbb{R}^{m \times n} \quad (3.6) \]

where the matrix \( S_p \) is simply the matrix \( S \) with the largest first \( p \) singular values kept and the smallest \( (n-p) \) singular values replaced by zeroes, and \( p \leq r \). Equation 3.6 can thus be inverted resulting in:

\[ A^{-1} = VS_p^{-1}U^T \quad (3.7) \]

where \( A^{-1} \) is called the pseudoinverse or Moore-Penrose inverse of \( A \) and

\[
S_p^{-1} = \begin{bmatrix}
1/\sigma_1 & 0 & \cdots & 0 \\
0 & 1/\sigma_2 & \cdots \\
& \ddots & \ddots & \vdots \\
0 & \cdots & 1/\sigma_p & 0 \\
0 & \cdots & 0 & 0
\end{bmatrix} \in \mathbb{R}^{n \times m}
\]

If there are no error considerations, the solution, \( x = A^{-1}y \) is the minimum norm solution to the problem \( y = Ax \) because:

\[
||A^{-1}y|| = \min \{ ||x|| \mid ||Ax - y|| = (1 - R)y|| \},
\]

where \( R \) is the projection onto the range of \( A \). However, in practice, the smallest positive singular values are very close to zero for an ill-conditioned matrix \( A \) and the minimum
norm solution is very sensitive to the errors in vector \( y \) resulting in a need to choose a truncation value, \( p \). To determine this truncation value, \( p \), assume the measurement vector \( y \) is a noisy approximation of the noiseless vector \( y_0 \) and with a measurement error, \( \eta \), the noise level can therefore be estimated as:

\[
||y - y_0|| \approx \eta, \quad \eta > 0
\]

The approximate solution therefore cannot have a smaller residual error than the measurement error, else we would be fitting the solution to the noise. Thus, in identifying the truncation parameter \( p \), we must find \( p \) such that \( 1 \leq p \leq m \) and the largest index satisfies the following criteria:

\[
||y - Ax_p|| = ||y - R_p y|| \leq \eta
\]

### 3.3.2 Inverse problem formulation

The mathematical model to retrieve the vertical skin SST profile from infrared emitted radiance spectra from the M-AERI was discussed in Section 3.2.2 and is defined by Equation 3.3. A numerical integration is first performed and Equation 3.3 can be rewritten as:

\[
I_m(v) = - \int_0^\infty B(v, T(z)) \frac{d(e^{-ax})}{dz} dz
\]

\[
I_m(v_j) \approx \sum_{i=1}^{n} w_i \cdot B(v_j, T(z_i)) \cdot \alpha_j \cdot (e^{-a_j z_i})
\]

(3.8)

where \( w_i \) and \( z_i \) are the weights and nodes of the quadrature rule respectively. For this study, we choose a 100-point Gauss-Legendre quadrature rule and an interval of integration -0.04 to 0 cm which allows for 20 unevenly spaced nodes to be within depths
of -0.01 to 0 cm. This interval may seem small, but as shown in Figure 3.6, this depth interval includes the source region for nearly all of the emitted IR radiation. A high resolution of 100-points is required because the skin layer depth scales are very small and a very accurate calculation of the integral is required to resolve the small changes in radiance values. Furthermore, because of the two different wavenumber regimes which are being used, the radiance values of \( I_m \) ranges widely from \( \sim 100 \ mW \ Sr^{-1} \ m^{-2} \ cm^{-1} \) at the lower wavenumber ranges, to \( \sim 1 \ mW \ Sr^{-1} \ m^{-2} \ cm^{-1} \) at higher wavenumbers.

A Taylor expansion of Equation 3.8 is subsequently performed assuming that we know a set of first-guess solutions: \( T_{1}^{fg}, T_{2}^{fg}, ..., T_{n}^{fg} \) at \( z_{1}, z_{2}, ..., z_{n} \). This results in:

\[
I_m(v_j) = I_f^g(v_j) + \sum_{i=1}^{n} \frac{\partial I(v_j)}{\partial T_i} |_{fg} (T_i - T_i^{fg})
\]  

(3.9)

where \( fg \) represents the first-guess solution and \( n \) is the number of irregularly spaced layers in which the thermal skin layer is divided by means of the quadrature rule. Comparing Equation 3.9 with \( y = Ax \), we are therefore solving the least squares problem:

\[
y_j = I_m(v_j) - I_f^g(v_j), \ j = 1, 2, ..., m
\]

\[
x_i = T_i - T_i^{fg}, \ i = 1, 2, ..., n
\]

\[
A_{ji} = \sum_{i=1}^{N} \frac{\partial I(v_j)}{\partial T_i} |_{fg}
\]

The first-guess solution is the erfc function, as described in Section 2.3
Chapter 4

Results

In this chapter, we present and discuss the simulation results obtained from the synthetic and field data runs for the thermal skin temperature layer profile retrievals. The synthetic data runs were performed with different first-guess profiles to give insight as to how the TSVD method operates and to allow for the proper techniques in the TSVD to be extended for the field data runs. Noise was also added to the synthetic data to obtain a more realistic simulation of field data. Errors were characterized and analyzed for both synthetic and field runs together with the determination of the truncation parameter.

4.1 Synthetic data results

4.1.1 Noiseless synthetic data results

To test the robustness and to validate the TSVD model, a set of synthetic data, $T_{original}(z)$, was generated using Equation 2.7 at $T_s = 301K$ and $T_b = 301.3K$. This profile, $T_{original}(z)$,
is taken be representative of the thermal skin layer and the aim is to retrieve this profile using our analysis technique. As described in Section 3.3, a set of first-guess profiles, $T_{fg}(z)$, is required in the TSVD model and 4 different first-guess profiles are generated as discussed in Section 2.3.2.

The results for all 4 cases are shown in Figures 4.1, 4.3 and 4.4. In case 1, the first-guess profile, $T_{fg}(z)$, is a very good approximation to the test profile, $T_{original}(z)$ and this gave results that are very close, having a mean-squared-error (MSE) of $3.97 \cdot 10^{-7} \text{K}^2$ and an error of $< 0.004 \text{K}$ (top panel of Figure 4.1). The use of a different first-guess solution in Case 2 produced a slightly worse solution with a MSE of $1.32 \cdot 10^{-5} \text{K}^2$. This is shown in the bottom panel of Figure 4.1, and the largest error deviation seen occurring is attributed to the discontinuity in the gradient in $T_{fg}(z)$ at $z = -0.02 \text{ cm}$. It is clear that this discontinuity is unphysical and is the result of the piece-wise linear structure of $T_{fg}(z)$ and that the TSVD approach is unable to resolve such structure.

An important conclusion can be made from the results of Cases 1 and 2: the form of the first-guess solution is important as the TSVD technique has a tendency to conform to a solution similar in shape to the first-guess. Thus, it is important to understand the possible theoretical forms of the thermal skin layer which has been previously described in Section 2.3.1. Since the thermal skin layer’s temperature profile is expected to be a smooth continuous function such as an erfc or exponentially decaying form as mentioned and experimentally measured by many, (eg. Katsaros et al. (1977); Spangenberg and Rowland (1961); Liu and Businger (1975)), taking Equation 2.7 to be a first-guess profile for retrievals using field data is expected to avoid unrealistic errors.
Figure 4.1: Left-hand graphs show a plot of depth versus temperature. Blue solid line: $T_{fg}(z)$ which is an erfc profile similar to $T_{original}(z)$ but with a change in the gradient; black solid line: $T_{original}(z)$; red dotted line: iterated result at $p=6$. Right-hand graphs show a plot of depth versus the errors between $T_{original}(z)$ and the iterated result. Upper graphs: Case 1 results; lower graphs: Case 2 results.
For both cases 1 and 2, the best MSE values happen at the truncation parameter of p=6. Table 4.1 shows the MSE value at p=6, the largest error and the depth at which the error occurs. A logarithmic plot of the singular values obtained shows that p=6 implies that there is a noise level of ~0.0001 (0.01%), (Figure 4.2). Thus, even though the synthetic data are error-free, there are still errors arising from the numerical integration calculations and the use of the TSVD approximation for a matrix that is very ill-conditioned (condition number ~ 1.3 · 10^{21}).

<table>
<thead>
<tr>
<th>Case</th>
<th>MSE at p=6</th>
<th>Largest Error</th>
<th>Depth of Largest Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>Case 1</td>
<td>3.97 · 10^{-7} K^2</td>
<td>0.00286 K</td>
<td>-0.00436 cm</td>
</tr>
<tr>
<td>Case 2</td>
<td>1.32 · 10^{-5} K^2</td>
<td>0.0146 K</td>
<td>-0.0203 cm</td>
</tr>
<tr>
<td>Case 3</td>
<td>2.78 · 10^{-3} K^2</td>
<td>0.0533 K</td>
<td>-0.0264 cm</td>
</tr>
<tr>
<td>Case 3: $T_b = T_{fg} + 0.07$</td>
<td>1.63 · 10^{-5} K^2</td>
<td>0.0145 K</td>
<td>0 cm</td>
</tr>
</tbody>
</table>

Table 4.1: MSE values at p=6, Largest error and the depth at which the error occurs for all cases.

For cases 3a and 3b, the intention was to start from the radiance spectra, $I_m(\nu)$, obtained by assuming $T_{original}(z)$ is the thermal skin layer measured by the M-AERI after atmospheric correction is performed, and simulate field data retrievals. In order to obtain a good first-guess profile, $T_{fg}(z)$, the BTs were obtained from $I_m(\nu)$ and mapped to the penetration, or emission, depth, $\frac{1}{D_p}$, as described in Section 3.2. Equation 2.7 is fitted to the depth versus BT profile obtained and is subsequently used as the first-guess solution. This method would imitate the situation when field data from the M-AERI are used without imposing $T_{original}(z)$. 
Figure 4.2: Logarithmic plot of the singular values of the discretized inverse problem, Equation 3.3, for synthetic data. The red solid line indicates the level of the machine epsilon ($2.2204e^{-16}$) and the red dotted line indicates the noise level of 0.0001 (0.01%).

Figure 4.3 shows the results of the run from case 3a. The results are not as favorable as in the first 2 cases and overshoots are seen at $p \geq 3$ which are clearly unphysical. Figure 4.3 illustrates the importance in the choice of the truncation parameter, $p$. Note that at $p=3$ and 4, the solution shows temperature inversions at depths of about -0.005 cm to -0.01 cm and oscillatory profiles are found for $p > 4$. This shows that invoking the direct mapping of depth to BT using Figure 3.6 causes solutions that are unable to converge on a realistic solution. The iterated solutions closest to $T_{original}(z)$ are at $p=3$ and $p=4$ which still results an undesirable inversion. An explanation of the inversions is that the $T_b$ of the iterated solutions are observed to converge to $T_{fg}^b$ and since $T_{fg}^b$ is smaller than $T_b$ of $T_{original}(z)$, the iterated solution attempts to compensate for this smaller value by having a larger temperature value in the iterated solution near the surface, resulting in an inversion. It seems that the $T_{bg}^f$ and $T_{fg}^b$ values play a very
Figure 4.3: Case 3a: Green: the retrieval assuming that the M-AERI is measuring a thermal skin layer profile, $T_{original}(z)$, represented by the black solid line. Blue dotted line: $T_{fg}(z)$ which is an erfc function fitted to the green; red lines: the iterated result at $p=3,4,5,6$.

important role in the convergence of the solution and must be as close to the $T_s$ and $T_b$ of $T_{original}(z)$ to avoid unphysical oscillations. To test this theory, case 3b was set-up in which $T_{fg}^{b}$ is incrementally increased to higher temperature values such that $T_{fg}^{b}$ would be close to the actual $T_b$. This occurred at $T_b = T_{fg}^{b} + 0.07$ and is shown in the lower panel of Figure 4.4 in which the iterated solution converges nicely to $T_{original}(z)$, resulting in a case similar to Case 1 at $p=6$. 
Figure 4.4: Left-hand graphs shows a plot of depth versus temperature. Green: the retrieval assuming that the M-AERI is measuring $T_{\text{original}}(z)$ represented by the black solid line. Blue solid line: $T_{\text{fg}}(z)$ which is an erfc function fitted to the green; red solid line: the iterated result at $p=6$. Right-hand graph shows a plot of depth versus the difference between $T_{\text{original}}(z)$ and the iterated result. Upper panel: Case 3a results; lower panel: Case 3b results with $T_b = T_{\text{fg}} + 0.07$. 
An additional test was performed to assess whether averaging radiance spectra would give better results. Eight profiles were generated at different $T_s$ values ranging from 300.3 K to 301 K in increments of 0.1 K with the same $T_b$ value of 301.45 K and averaged to obtain $T(z)$. The radiance spectra for each of the 8 profiles were subsequently calculated using a trapezoidal rule and also averaged. This averaged radiance spectrum was used to retrieve a temperature profile using conditions from Case 3b and it was found that the retrieved temperature profile converged to the averaged profile $T(z)$ (Figure 4.5). This shows that averaging radiance spectra would indeed give the average temperature profile.

It is important also to note the difference in radiances of each of the 8 profiles with respect to the averaged profile $T(z)$ (bottom panel of Figure 4.5). The differences are about 100 times smaller than the magnitude of the radiances. This illustrates the difficulty in retrieving a temperature profile of the problem from measurements that include noise, as it means that the least squares fit using the TSVD must be obtained from accurate radiance spectra with a noise level small enough for the signal to not be masked.
Figure 4.5: Top panel shows eight temperature profiles (blue and cyan lines), the average of the 8 generated profiles (green line), the first-guess using conditions from Case 3b (pink line) and the retrieved profile using the averaged radiances of the 8 generates profiles (black dotted line). Bottom panel shows the difference in radiance values of each of the 8 temperature profiles with respect to the averaged.
4.1.2 Noise-added synthetic data results

The cases above were all performed without noise, however, sea-going measurements of the M-AERI contain noise. Thus, randomly distributed noise was added to the spectral radiance of $T_{\text{original}}(z)$. The noise injected has a normal distribution which follows the M-AERI’s noise equivalent delta radiance (NEΔL) of 0.2 mWsr$^{-1}$m$^{-2}$cm$^{-3}$ and 0.015 mWsr$^{-1}$m$^{-2}$cm$^{-3}$ at wavenumbers 670-1400 cm$^{-1}$ and 2000-2600 cm$^{-1}$ respectively. A sample retrieval of the temperature profile was attempted using conditions from Case 3b and is shown in Figure 4.6. It is clear that noise in the radiance values causes the BT values to have a much larger variations. The retrieved profile is therefore affected by the large BT variation preventing convergence to the desired profile.
Figure 4.6: Sample run with noise added to the radiance spectrum of $T_{\text{original}}(z)$. Left-hand graph shows a plot of depth versus temperature. Green: the retrieval assuming that the M-AERI is measuring $T_{\text{original}}(z)$ with noise added to the radiance spectrum; black line: $T_{\text{original}}(z)$ without noise; blue line: $T_{\text{fg}}(z)$ which is an erfc function fitted to the green crosses with $T_b = T_{\text{fg}}^b + A$, where A is a constant. This line happens to overlaid by the red solid line; red solid line: the iterated result at $p=2$. Right-hand graph shows the difference between $T_{\text{original}}(z)$ and the iterated result.
To minimize the errors caused by the noise, an averaging of radiance values were done for every 40 cm$^{-1}$ at the lower wavenumber range of 800-1200 cm$^{-1}$ and because of the large variability seen at the higher wavenumber range of 2640-2800 cm$^{-1}$ due to the higher dependency and variability on derived emissivity values, this entire range was averaged into one point. This gives 10 points at the lower wavenumbers and 1 point at the higher wavenumbers (Figure 4.7). The TSVD was applied to these 11 points and the results of 5 individual runs in which each run has random normally distributed noise injected into the radiance spectrum are shown in Figure 4.8. The results show that the retrieved profile converges to the desired profile but with some slight discrepancies mainly in the sub-skin temperature value. A possible reason for this is that because of the high variability of BT at deeper depths, the averaged point also has a much higher variation. Despite the variation in $T_b$, a smooth profile can be retrieved with a curvature similar to the original profile.
Figure 4.7: Sample dataset of temperature versus depth with noise added to the radiance spectrum of $T_{\text{original}}(z)$. Black stars represent the averaging of the radiance values with 10 averaged points for the shallowest BT values and 1 averaged point for the deeper BT. Black line represents the best fit erfc curve through the 11 points.
Figure 4.8: Five sample retrievals with noise added to the radiance spectrum of $T_{original}(z)$. Green crosses: 11 averaged points from the noisy BT plot; black line: $T_{original}(z)$ without noise; blue line: $T_{fg}(z)$ which is an erf function fitted to the green crosses with $T_b = T_{fg} + A$ where A is a constant; red line: iterated result at p=2.
4.2 Field data results

Building on the findings from the synthetic data runs, 300 individual radiance spectra were processed from the AMMA2006 cruise, averaged and used as a dataset for the assessment of the TSVD approach on field data. The conclusions obtained from the synthetic data runs were extended to this cruise dataset and the results are discussed in the second section. The first section describes how the truncation parameter is determined by using knowledge of the signal-to-noise ratio of the M-AERI.

4.2.1 Truncation parameter determination

The M-AERI has the smallest signal-to-noise ratio (SNR) of 135 at 3000 $cm^{-1}$ (Minnett et al. (2001)) with better SNR values of 1800 at lower wavenumbers. Thus the largest fractional uncertainty is 0.0074 and this was rounded up to 1% to be used as the error value to determine the level of truncation. Figure 4.12 shows the logarithm plot of the singular values obtained from the field data and a noise level of 1% is illustrated by the dotted red line. The logarithmic plot shows that a truncation parameter of $p=3$ ought to be chosen.

<table>
<thead>
<tr>
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<th>4</th>
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<td>Singular Value, S</td>
<td>2.9645</td>
<td>0.1825</td>
<td>0.0256</td>
<td>0.0067</td>
<td>0.0014</td>
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<tr>
<td>Log(S)</td>
<td>1.09</td>
<td>-1.70</td>
<td>-3.67</td>
<td>-5.01</td>
<td>-6.57</td>
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<td></td>
<td>6</td>
<td>7</td>
<td>8</td>
<td>9</td>
<td>10</td>
</tr>
<tr>
<td>Singular Value, S</td>
<td>$2.21 \cdot 10^{-4}$</td>
<td>$6.81 \cdot 10^{-5}$</td>
<td>$7.07 \cdot 10^{-6}$</td>
<td>$2.23 \cdot 10^{-6}$</td>
<td>$1.79 \cdot 10^{-7}$</td>
</tr>
<tr>
<td>Log(S)</td>
<td>-8.42</td>
<td>-9.59</td>
<td>-11.86</td>
<td>-13.01</td>
<td>-15.54</td>
</tr>
</tbody>
</table>

Table 4.2: Table of the first 10 singular values in Figure 4.12 and their logarithmic values.
Figure 4.9: Logarithmic plot of the singular values of the discretized inverse problem, Equation 3.3 using M-AERI data obtained from the AMMA2006 cruise. The red solid line indicates the level of the machine epsilon ($2.2204e^{-16}$) and the red dotted line indicates the noise level of 0.01 (1%).

Shown also in Table 4.2 are the first 10 singular values from Figure 4.12. In order for the truncation to be performed at a level of $p=3$, we see that the fractional uncertainty, $\Psi$, needs to be in the interval: $0.0067 < \Psi < 0.0256$ or $0.67\% < \Psi < 2.56\%$ which translates to an instrument's SNR range of $39.0 < \text{SNR} < 149.2$. This truncation level works well for the cruise spectra as oscillatory profiles are seen for $p \geq 4$, which result from numerical instabilities. Also from Table 4.2, we see that in order to increase the accuracy of the retrieval to a level similar to the synthetic data runs ($p=6$), a range of $\Psi < 2.21 \cdot 10^{-4}$ or $\text{SNR} > 4520$ is desired.
When the iteration was performed, truncating the singular value matrix at $p=3$ indeed works well (Figure 4.10). High oscillatory profiles similar to Figure 4.3 are immediately seen occurring at $p \geq 4$.

### 4.2.2 Iterated results

From the results of the synthetic data analysis, an inversion is expected to occur at depths of around -0.005 cm if the value $T_{bg}^{fg}$ is not incremented to higher values. The top panel of Figure 4.10 shows that this is true and agrees well with our expectations. Comparing Figure 4.10 with Figure 4.3 from case 3a of the synthetic runs tells us that the inversion seen is likely to be unphysical and there is a need to increment $T_{bg}^{fg}$. The bottom panel of Figure 4.10 shows the result when $T_{bg}^{fg}$ is incremented in intervals of 0.01 K until the inversion disappears; this happened at the point $T_b = T_{bg}^{fg} + 0.1$. It is also interesting to note that a very smooth profile (red) is obtained and is close to that of the first-guess solution (blue). Different first-guess profiles with the same $T_s$ and $T_b = T_{bg}^{fg} + 0.1$ but a different gradient were also used and observed to converge to the same profile, indicating that the solution is robust.

The percentage difference in radiance values, $\frac{B(v, T(z)) - I_m}{I_m} \cdot 100\%$, between the first-guess and iterated solution when $T_b = T_{bg}^{fg} + 0.1$ is shown in the top panel of Figure 4.11. There is no significant change in this difference at the higher wavenumbers since there is not a big change in the temperature profile at deeper depths of $< -0.01 \text{ cm}$. The curvature adjustment at shallow depths of $> -0.01 \text{ cm}$ has resulted in a reduction in the percentage error of the radiances at the lower wavenumbers.
Figure 4.10: Temperature profiles; blue line: $T_{fg}^b(z)$ which is an erfc function fitted to the M-AERI spectra represented by the green crosses; red line - iterated result at $p=3$. Top panel: $T_b = T_{b_{fg}}$; bottom panel: $T_b = T_{b_{fg}} + 0.1$. 
Shown also in the bottom panel of Figure 4.11 is the percentage difference in radiances between the measured M-AERI spectral data and both iterated results from Figure 4.10. Both lines are observed to be very close. In other words, the TSVD method of obtaining a least squares fit to the spectral radiances would not help in determining whether the retrieved profile is 'true'. The reasons for rejecting the iterated solutions with the inversions are firstly because of the unphysicality seen from the synthetic profile runs and secondly, in theory, such a large inversion in the temperature gradient could not be supported in such a thin layer as molecular conduction would remove the heat down the temperature gradient in both upward and downward directions. Thus, even if such an inversion were to occur it would quickly decay to a profile similar to the bottom panel of Figure 4.10. This is discussed further in Chapter 5.

The three hundred averaged profile runs from the AMMA cruise indicate that the algorithm works. However, given that under normal operations, a M-AERI measurement sequence takes ~ 12 minutes, only five spectra are taken per hour. Thus, averaging three hundred profiles means that the retrieved thermal skin layer is an average of 60 hours, which takes about five days to accumulate as only night time data can be used. This is not desired as the main objective is to link the thermal skin layer’s curvature with heat fluxes and thus ideally requires the retrieval from individual spectra, or an average over a small number of spectra. When individual profile retrievals were attempted, the noise in the spectra caused the TSVD algorithm to not converge. Thus, the technique of averaging the radiance values into 11 points (as discussed in the synthetic data runs) was adopted. The truncation was performed at p=2, as there are
Figure 4.11: Plots of the difference in radiances with the measured M-AERI spectral radiance as a percentage. Top panel: radiance difference of the first-guess radiances (blue line); radiance difference of the iterated result’s radiances at $p=3$ (red line). Bottom panel: radiance difference where no inversion exists in the iterated solution (black line); radiance difference where an inversion exists in the iterated solution (green line).
only 11 singular values, due to the 11 points in the dataset. Ten sample individual profiles are shown in Figure 4.13. All the retrievals show smooth continuous profiles and the number of iterations ranged from 1 iteration performed for profiles with yearday 148.0467 and 193.0436, to 38 iterations for yearday 162.955. Each iteration meant incrementing $T_{fgb}$ by 0.01 K and the criterion for the algorithm to exit is that no further gradient change in the resultant profile is found. Figure 4.14 shows a flowchart of the algorithm used. Typical differences in radiance values at the higher wavenumbers are $< 0.01 \text{mW sr}^{-1}\text{m}^{-2}\text{cm}^{-1}$ and at lower wavenumbers $< 0.2 \text{mW sr}^{-1}\text{m}^{-2}\text{cm}^{-1}$.

![Graph](image)

**Figure 4.12:** Logarithmic plot of the singular values of the discretized inverse problem, Equation 3.3 using a M-AERI spectrum obtained from the AMMA2006 cruise. The red solid line indicates the level of the machine epsilon ($2.2204 \cdot 10^{-16}$) and the red dotted line indicates the noise level of 0.01 (1%).
Figure 4.13: Ten sample profiles derived from spectra taken during the AMMA 2006 cruise.
Remove reflected atmospheric radiance

Average radiance spectra into 10 wavenumber intervals of 40 cm\(^{-1}\) from wavenumbers 800 - 1200 cm\(^{-1}\) and 1 wavenumber interval from wavenumbers 2640 - 2800 cm\(^{-1}\)

Calculate BT of the 11 averaged radiance values and perform mapping to \(D_p\) to generate temperature versus depth profile

Generate First-Guess using erfc fitted to the 11 BT values

Perform TSVD and truncate at \(p = 2\)

Is an inversion observed in the retrieved profile?

yes

Increment \(T_b\) by 0.01 K and shift \(T_s\) to \(T_s\) of the retrieved profile

Generate first-guess using the new \(T_b\) and \(T_s\) values

no

Figure 4.14: Flowchart of algorithm using 11 radiance values and incrementing \(T_b\) by 0.01 K.
From Sections 4.1 and 4.2, the results obtained clearly indicate that the solution to the inverse equation is not unique and results in the generation of different profiles with very similar error magnitudes. Therefore, how do we know which solution profile is closest to the true profile? The oscillatory solutions are obviously not physical since it is not possible to support multiple large gradient reversals in such a thin layer and these oscillations are due to the ill-conditioning of the inverse problem. However, the retrieval done with M-AERI data has shown to display an inversion at depths of \(~0.05 \text{ mm} - 0.1 \text{ mm}\) for the case when $T_b$ is not shifted to a higher value (Figure 4.10). Even though this has been deemed unphysical from the results obtained from synthetic data runs (Figures 4.3 and 4.4), it is still important to understand the possibility of such a gradient reversal occurring in the thermal skin layer. Section 5.1 gives a brief background on this gradient reversal previously observed by others in experiments, following which the dimensionless Rayleigh number is analyzed at our depths of interest. The last section describes a simple experiment to test the possibility of a gradient reversal occurring at depths of the thermal skin layer due to sea surface renewal effects.
5.1 Background on the existence of a gradient reversal in the skin SST layer

It is interesting to note that some previous studies performed on the thermal skin layer noticed inversions while others did not. Chu and Goldstein (1973) and Herring (1963) who were studying turbulent thermal convection of water between two parallel plates observed inversions, together with Veronis (1966) and Chang and Wagner (1975) who were studying Bénard convection and changes in surface temperatures due to small amplitude surface waves observed these inversions. On the other hand, Katsaros et al. (1977) performed an experiment in an open tank of water and did not observe the inversions, nor did Spangenberg and Rowland (1961) who had done a similar experiment to study natural convection in water, or Ward et al. (2004) using an upper decameter SST profiling instrument called SkinDeEP. Even numerical simulations of free convection done by Leighton et al. (2003) did not find inversions. Katsaros did state the studies which observed the inversions, or 'knees', to be unrealistic in their experimental conditions and summarized that these studies were obtained at Rayleigh numbers of less than $10^7$. She also confirmed the finding by Chu and Goldstein (1973), that for gradient reversals in the water to occur, an upper limit Rayleigh number of $\sim 8 \cdot 10^6$ is required and this requirement has some dependency on the Prandtl number. Furthermore, the presence of inversions are also noted to occur in earlier studies and at depths below the skin layer while the later and more recent studies, with improved instrumentation, did not show the presence of these inversions.
Despite this, none of the studies (including the more recent ones) are concentrated on the upper layers of the skin layer profile of less than 1 mm as most of the studies are performed at centimeter scales due to instrumental limitations and capabilities. At depths of a few centimeters, the Rayleigh numbers are much larger and the analysis of the thermal skin layer has been extended into the sub-skin SST layer. The millimeter depth scales of the thermal skin layer which are of interest are not entirely applicable to the studies presented in these papers and experience a completely different mechanism. Furthermore, the gradient reversals seen by Chang and Wagner (1975) occur at a depth of \(~1\) cm with a temperature difference of 0.04 K with respect to the bulk temperature, while Chu and Goldstein (1973) observed a reversal occurrence at 3.8 mm with a temperature difference of about 0.25 K. Both of which are away from the skin SST boundary layer and are deeper than the inversions observed for our M-AERI retrievals.

5.2 The Rayleigh number and molecular conduction in the skin SST layer

For further discredit of the possibility of an existence of a temperature inversion in the thermal skin layer, one concept is to show that molecular conduction is the dominant phenomenon happening at the skin layer depths. Molecular conduction is an efficient method of heat transfer and occurs when there is a temperature gradient across a medium (which in this case is water). Energy is transferred from a high temperature
region to a low temperature region due to random molecular motion. Thus, if an inversion or maximum temperature, \( T_{\text{max}} \), were to occur, as in the top panels of Figure 4.10 and Figure 4.3, this temperature would be expected to quickly decay to a value of the sub-skin temperature resulting in a smooth continuous profile as in the bottom panel of Figure 4.10.

A simple way to determine whether the dominant phenomenon is conduction or convection is to look at the dimensionless Rayleigh number. The Rayleigh number, \( R_a \), can be understood as the ratio between the rate of heat transfer by convection to the rate of heat transfer by conduction. This dimensionless number exhibits the form:

\[
R_a = \frac{bgL^3dT}{\alpha \nu}
\]  

(5.1)

where \( g \) is the gravitational constant, \( b \) equals to the coefficient of thermal expansion, \( L \) is the length scale, \( dT \) is the temperature difference across length \( L \), \( \alpha \) is the thermal diffusivity and \( \nu \) is the viscosity of the medium. The effects of salinity variations on density are small and can be ignored.

Analytically, Lord Rayleigh, (Rayleigh, 1916), saw that there is a finite value of the temperature difference, \( T_c \), for the onset of convection, and predicted that a critical Rayleigh number, \( R_{ac} \), of \( \frac{27\pi^4}{4} \) is required for convection to occur assuming there was free slip between the fluid and the boundaries. Jeffreys (1926) predicted a \( R_{ac} \) value of 1709 for a fluid confined between two horizontal boundaries with no slip between the boundary and fluid while Low (1929) predicted a \( R_{ac} \) of 1108 if one of the boundaries is rigid while the other is free. Experimentally, Spangenberg and Rowland (1961)
obtained an estimated $R_{ac}$ of 1193 for the onset of natural convection to occur and a $R_{ac}$ of 102 for this convection to be maintained in an experimental tank. They also observed that convection did not occur at water depths of less than 1cm.

We explored the Rayleigh number at dimensions of skin layers depths. The Rayleigh number was first calculated at a temperature difference range of 0.1 - 1.0 K at a length scale of 1 mm and 0.1 mm, i.e. characteristic of the thermal skin layer. This is shown in Table 5.1. We see that the maximum Rayleigh number, 16.41, occurs for a temperature difference of 1 K. This is very small compared to the $R_{ac}$ values for convection and confirms that the mean temperature gradient in the skin layer can exist without being disrupted by convection.

<table>
<thead>
<tr>
<th>$\Delta T$</th>
<th>0.1 K</th>
<th>0.2 K</th>
<th>0.3 K</th>
<th>0.4 K</th>
<th>0.5 K</th>
<th>0.6 K</th>
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</thead>
<tbody>
<tr>
<td>Depth=1 mm</td>
<td>1.64</td>
<td>3.28</td>
<td>4.92</td>
<td>6.56</td>
<td>8.2</td>
<td>9.85</td>
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<tr>
<td>Depth=0.1 mm</td>
<td>0.00164</td>
<td>0.00328</td>
<td>0.00492</td>
<td>0.00656</td>
<td>0.00820</td>
<td>0.00985</td>
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<table>
<thead>
<tr>
<th>$\Delta T$</th>
<th>0.7 K</th>
<th>0.8 K</th>
<th>0.9 K</th>
<th>1.0 K</th>
</tr>
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<tbody>
<tr>
<td>Depth=1 mm</td>
<td>11.49</td>
<td>13.13</td>
<td>14.77</td>
<td>16.41</td>
</tr>
<tr>
<td>Depth=0.1 mm</td>
<td>0.0115</td>
<td>0.0131</td>
<td>0.0148</td>
<td>0.0164</td>
</tr>
</tbody>
</table>

Table 5.1: Table of Rayleigh values at length scales of 1 mm and 0.1 mm for a range of temperature differences.

An $R_{ac}$ of 1193 and 102 as predicted by Spangenberg and Rowland (1961) were subsequently assumed to calculate the length scales required to meet the minimum $R_{ac}$ value (Table 5.2). A minimum of 4 mm is required for the onset of convection to occur and a minimum of 1.83 mm is required to maintain convection. These values are larger than our skin layer depths of 0.1-1 mm and thus convection is not occurring at these depth scales. As an additional reference, the range of length scales required for a $R_{ac}$
of \(\frac{27\pi^4}{4} = 657.5\) are shown in Table 5.2. This simple analysis confirms that depths of \(\sim 1 \text{ mm}\) beneath the ocean-atmosphere interface are laminar. Reversals in temperature gradients cannot be supported at depths of about 1 mm as molecular conduction, being a very efficient method of heat transfer, would quickly erode temperature inversions resulting in a smooth continuous profile.

<table>
<thead>
<tr>
<th>(\Delta T)</th>
<th>0.1 K</th>
<th>0.2 K</th>
<th>0.3 K</th>
<th>0.4 K</th>
<th>0.5 K</th>
<th>0.6 K</th>
</tr>
</thead>
<tbody>
<tr>
<td>(R_a = 102)</td>
<td>3.96 mm</td>
<td>3.14 mm</td>
<td>2.75 mm</td>
<td>2.50 mm</td>
<td>2.32 mm</td>
<td>2.18 mm</td>
</tr>
<tr>
<td>(R_a = 1193)</td>
<td>8.99 mm</td>
<td>7.14 mm</td>
<td>6.23 mm</td>
<td>5.66 mm</td>
<td>5.26 mm</td>
<td>4.95 mm</td>
</tr>
<tr>
<td>(R_a = 657.5)</td>
<td>7.37 mm</td>
<td>5.85 mm</td>
<td>5.11 mm</td>
<td>4.64 mm</td>
<td>4.31 mm</td>
<td>4.06 mm</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>(\Delta T)</th>
<th>0.7 K</th>
<th>0.8 K</th>
<th>0.9 K</th>
<th>1.0 K</th>
</tr>
</thead>
<tbody>
<tr>
<td>(R_a = 102)</td>
<td>2.07 mm</td>
<td>1.98 mm</td>
<td>1.90 mm</td>
<td>1.83 mm</td>
</tr>
<tr>
<td>(R_a = 1193)</td>
<td>4.70 mm</td>
<td>4.50 mm</td>
<td>4.32 mm</td>
<td>4.17 mm</td>
</tr>
<tr>
<td>(R_a = 657.5)</td>
<td>3.85 mm</td>
<td>3.69 mm</td>
<td>3.54 mm</td>
<td>3.42 mm</td>
</tr>
</tbody>
</table>

Table 5.2: Table of minimum depth values required assuming Rayleigh numbers of 102, 1193 and 657.3.

### 5.3 Sea surface renewal effects in the skin SST layer

This experiment is to examine the likelihood of the formation of the temperature gradient reversal due to convection arising from sea surface renewal effects. Sea surface renewal theory describes the phenomenon of convective cells with Kolmogorov length scales happening near the surface of the water. This type of convection is also commonly known as the Rayleigh-Bénard convection whose effect is due to the presence of a temperature gradient. Rising parcels of warm water starting at depths of the bottom of the sub-skin SST layer (or slightly deeper), hits the bottom boundary of the thermal
skin layer in which a large temperature gradient change occurs, spreads out, and eventually cools from evaporation, sensible heat loss and infrared emission and converging into thin narrow regions of downwelling. This type of convection has been shown and proven experimentally to exist by many (e.g. Spangenberg and Rowland (1961); Chang and Wagner (1975)). Due to the spreading of the warm parcel of water, a skewness is seen in the spatial temperature distribution towards warmer temperatures from these sea surface renewal effects. This is seen in an experiment in which images of the water surface from an IR camera were taken in the Air-Sea Interaction Saltwater tank (ASIST) at RSMAS. The IR camera used was from the FLIR Systems High Performance Thermal Imaging System SC 3000 which measured in the spectral range of 8-9 $\mu$m and has a thermal image relative accuracy of 0.02 K. The air-sea temperature difference, $\Delta T$, ranged from -15 K to 15 K with the negative sign denoting that the water is warmer than the air and wind speeds were varied from 0 m/s to 10 m/s. A skewness towards warmer temperatures was seen and the corresponding histograms are shown in Figures 5.1 and 5.2 for a $\Delta T$ of -15 K with wind-speeds of 0 m/s and 4 m/s.

Since the M-AERI is taking a spatially averaged reading in an area of about 1 m$^2$, it is interesting to explore whether this skewness towards warmer SSTs may potentially cause the averaged skin layer profile retrieved from the M-AERI to experience a reversal in the temperature gradient. To test this theory, an estimate of each instantaneous depth versus temperature profile was made. Referencing to the 0 m/s wind-speed experimental runs, an isothermal 'neutral' profile of 313.5 K was assumed. Profiles with a surface temperature above 313.5 K are termed 'warm-profiles' while those with a surface temperature of below 313.5 K are termed 'cold-profiles'. The cold-profiles were
Figure 5.1: Infrared Image (top) and histogram (bottom) of sea surface temperature for an air-sea temperature difference of -15K and wind speed of 0 m/s.
Figure 5.2: Infrared Image and histogram (bottom) of sea surface temperature for an air-sea temperature difference of -15K and wind speed of 4 m/s.
estimated by scaling the 'cold plunging plume' profile results at steady state from Span-gebenberg and Rowland (1961). The 'warm-profiles' were estimated by assuming that the rising parcel of warm water decrease in thickness at a rate of 0.1 K/mm, starting at a depth of 10 mm and at a maximum temperature of 314.5 K. All profiles included a skin effect of 0.02 K. The profiles are shown in Figure 5.3.

Each instantaneous profile was subsequently weighted according to the histogram and averaged. The resultant profiles are shown as the black dotted-dashed line in Figures 5.2 and 5.3. It is interesting to note that, an inversion is obtained at a depth of about 2 mm with a temperature difference of about 0.05 K. Even though this was a very rough estimate, comparing it to experimental studies by Chang and Wagner (1975) and Chu and Goldstein (1973), the results compares respectably well with Chu and Goldstein (1973) observation of 0.25 K at 3.8 mm. However, it is important to stress again that these observations are still below the boundary layer of the thermal skin layer and observations of temperature-depth profiles below 1 mm still exhibit smooth, continuous and laminar profiles without temperature gradient reversals.
Figure 5.3: Instantaneous profiles estimated (blue lines) and weighted profile (black dotted-dashed line) with respect to the Infrared image corresponding to a wind speed of 0 m/s. Top image shows all the instantaneous profiles estimated and the average weighted profile. Bottom image shows a magnification of the average weighted profile.
Although the skin SST has been recognized as an important parameter in climate studies and air-sea interactions, knowledge of the parameter is not well understood. The need for a better understanding of the physics of the thermal skin layer is driven by the desire for higher accuracy SST measurements, particularly from satellites, and understanding the warming of the ocean by greenhouse gases which is hypothesized to be related to changes in the gradient of the thermal skin layer. The M-AERI was used in the retrievals of the thermal skin layer temperature profile, however, due to the ill-conditioning of the inverse problem associated with the M-AERI measurements, there is a need to adopt regularization techniques.

This study has demonstrated the use of a well-known regularization technique called the Truncated Singular Value Decomposition (TSVD), as a method to retrieve the temperature profile of the thermal skin temperature layer using spectral radiance data obtained from the M-AERI. Before the TSVD could be used, field data from the M-AERI must be corrected for the reflected atmospheric radiance which requires knowledge
of the spectral emissivity values of the seawater. The VarMinT technique was demonstrated to be robust in determining the emissivity values required but the technique requires good contrast between the upwelling and downwelling measured radiances so that a good estimate of the emissivity values could be obtained since the technique utilizes the concept of minimizing the atmospheric component in the sea-view measurements. The sensitivity of emissivity to brightness temperature was also analyzed and seen to be more significant and variable at the higher wavenumbers due to the lower emissivity values and increasing sensitivity of radiance to brightness temperature with increasing wavenumber in the IR region.

The analysis of skin temperature profiles from synthetic data using the TSVD approach showed that knowledge of the first-guess profile is important and in particular, the surface temperature, $T_s$, and sub-skin temperature, $T_b$ of the first-guess must be close to the thermal skin layer’s surface and sub-skin temperature in order to retrieve the desired profile. The erfc function obtained from Liu and Businger (1975) was shown to be a good first-guess profile when field data are used as a smooth first-guess function is desired to avoid unrealistic errors formed by discontinuities in the first-guess profile. However, the linear mapping of penetration depth to brightness temperature with respect to wavenumber showed that there is a tendency of the sub-skin temperature, $T_b$, of the retrieval to be under-estimated resulting in inversions in the skin SST profile. Thus, there is a need to increase the first-guess, $T_b^{f_g}$, to obtain a better estimate of $T_b$ and remove the inversion artifact. Using the TSVD for the set of synthetic data also led to a noise level of 0.01% which results in a truncation parameter, $p=6$. When noise was added to the radiance spectrum, a large variability in the brightness
temperature resulted in the need to average the radiance spectra into 11 wavenumber intervals in order for the retrieval to be successful.

Applying the TSVD method to a three hundred averaged spectra from the M-AERI from the AMMA cruise, a truncation level of $p = 3$ was established for the M-AERI’s SNR, but unphysical inversions were found; these were removed by incrementing $T_b$ in the first-guess profiles. Individual profile retrievals were subsequently performed with the requirement of averaging the radiances into 11 wavenumber intervals and truncating at $p = 2$. Temperature inversions were also seen but removed by incrementing $T_{b}^{fg}$ with each iteration resulting in smooth continuous profiles. Removal of the inversion is further justified by computing the Rayleigh number which shows that the depth and temperature difference scales which are being analyzed here are laminar and dominated by molecular conduction, thereby implying that the reversal in the temperature gradient cannot be supported at these depths. A simple analysis to evaluate whether skewness in the distribution of temperature towards warmer temperatures that arise from sea surface renewal effects seen in thermal images may potentially support the temperature inversion, showed that such an inversion may exist but at sub-skin layer depths. Analysis of previous studies on the thermal skin layer also showed that inversions seen are at deeper depths of a few cm and no temperature gradient reversal observations were made at depths of $< 0.1\text{mm}$, i.e. within the skin layer.
In summary, the use of the TSVD method has been shown to produce the retrievals of the thermal skin layer temperature profiles using spectral radiance data obtained from the M-AERI. This is very encouraging for the future application of measurements from sea-going spectral radiometers, as instruments not only for the validation of satellite-derived SST but also for studying the physics of the ocean skin temperature layer. Understanding the gradient of the skin SST profile would also allow us to understand how greenhouse gases warm the ocean. Finally, the results of this study would provide increased knowledge and insights into processes involved with heat fluxes and climate change.
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