

New approach to remote sensing of temperature and salinity in natural water samples

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Abstract: Raman spectra for a natural water sample have been comprehensively investigated as a function of temperature and salinity, and we demonstrate that temperature and salinity can be determined from Raman spectra with RMS errors consistently below ± 0.2 °C and ± 0.6 PSU respectively where there is variation only in one parameter. Most significantly, we have applied multivariate methods to show that both temperature and salinity can be determined simultaneously from Raman spectra with RMS errors of ± 0.7 °C and ± 1.4 PSU respectively, and designed a three-channel Raman spectrometer that will be used for future studies.

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References and links

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1. Introduction

There are numerous fields that would benefit from a method for systematically mapping water temperature and salinity as a function of depth. Such information could be used to provide inputs to validate hydrologic modeling of water circulation, to provide habitat information about plant/animal species in waterways, understand the precursor conditions for algal blooms and to optimize underwater communications. From a climate change perspective, salinity and temperature profiles are critical parameters, and the direct measurement capability proposed here could enable modeling to be validated and improved. While passive satellite technology enables monitoring of sea surface properties, there is currently no standard method for measuring subsurface water temperature and salinity, other than the use of expendable probes or submersing strings of thermocouples. Here we report a new approach to rapid depth-resolved mapping of water temperature and salinity profiles, which we anticipate will be compatible with surface, subsurface or airborne platforms.

It is well known that both water temperature and salinity alter the Raman spectra of ocean water [1–3]. Both of these physical parameters produce subtle but distinct changes to the OH Raman stretching band (2800–3800 cm^{-1}). Significant differences are also observed between Raman spectra acquired from fresh and saline water due to the influence of various salt ions bonding into the water structure which modifies the molecular vibrations, affecting OH bond vibrational transition frequencies, and altering spectral shapes and polarization behavior [4]. Accordingly, there is a basis for harnessing this temperature and salinity-dependent behavior in order to predict the temperature and salinity of a water sample from its measured Raman spectra.

Raman spectroscopy was first applied to remotely sense water temperature in the 1970s, with detailed investigations by Chang and Young [5] and Leonard et al. [6], who proposed the so-called two-color method, in which Raman-scattered light is analyzed to measure the ratio of amplitudes corresponding to the two main peaks in the spectra, this ratio being found to vary linearly with temperature. They also proposed a depolarization method in which the Raman signal is separated according to polarization and the ratio of emission intensities for orthogonal polarization states is measured. In more recent times, similar research has continued, with the most recent work by Oh et al. [7] finding that water temperature could be predicted with an accuracy as high as ± 0.2 °C. Our own work has identified the spectral parameters (regions) most sensitive to temperature, and those which give rise to the most accurate determination of temperature [8]. We then used those findings to design a two-channel Raman spectrometer that could predict the temperature in a 1m long cell of water to an accuracy of ± 0.5 °C.

There has been much less effort devoted to Raman remote sensing of salinity. To our knowledge, the only attempts are reported in [9, 10] where an Artificial Neural Network was applied to solve the inverse problem of determining temperature and salinity using the shape of the valence band for a variety of natural water samples. The authors reported that their initial results resulted in mean absolute errors of below ± 0.5 °C for temperature and ± 0.7 practical salinity units (PSU) for salinity. This method however is not well-suited to depth resolved measurements, as it requires the collection of full Raman spectra.

Our goal has been to build on previous work by ourselves and others, and develop a viable approach to rapid depth-resolved mapping of water temperature and salinity profiles, which we anticipate will be compatible with surface, subsurface or airborne platforms. To this end, we present unpolarized Raman spectra obtained for samples of water from Sydney Harbour which exhibit systematic dependence on water temperature and salinity, and demonstrate how these can be decoupled through the use of multivariate analysis techniques. Numerical models based on multiple linear regressions indicated that for this particular water sample, temperature and salinity could be predicted with RMS errors below ± 0.6 °C and ± 1.2 PSU respectively. Furthermore we propose and simulate the performance of a simple three-channel optical system

that could (in the future) be used to measure integrated Raman signals over 100 cm^{-1} wide bands, finding that temperature and salinity could be predicted with RMS errors of $\pm 0.7\text{ }^{\circ}\text{C}$ and $\pm 1.4\text{ PSU}$.

2. Experimental details

Seawater samples were obtained from the Macquarie University Seawater Facility, which stores filtered seawater collected from Rose Bay, which is in the outer part of Sydney Harbour. These were diluted with de-ionized Millipore water ($18.2\text{ M}\Omega$ at collection) to provide samples having a range of salinity levels; these were measured using a conductivity probe (Extech EC600), and had an uncertainty of 1.5% of the full range. Each successive dilution and conductivity measurement was conducted directly prior to sample analysis. Conductivity values were converted to the Practical Salinity Scale, following the method in [11]. This scale is based on a ratio of measured conductivity against a potassium chloride reference sample at a specific temperature. The experiment was conducted over several days, and fresh water from the storage facility was obtained each day. The salinity of the filtered seawater (32.4 PSU) was slightly lower than average ocean salinity (35 PSU), but it was not possible to increase the salinity without losing some proportion of the dissolved salt content.

Raman Spectra were collected using a dispersive Raman spectrometer (Enwave EZRaman-I) which has a spectral resolution of $\sim 8\text{ cm}^{-1}$, and uses a frequency-doubled, linearly polarised, CW Nd:YAG laser (30 mW at 532 nm) for excitation. The signal detection path was collinear with excitation, i.e. the 180° backscattered Raman signal was collected, and polarisers could be introduced into the Raman signal beam path to obtain polarised spectra, i.e. the Raman signals having polarisation parallel or orthogonal to the polarisation of the excitation laser. Wavelength calibration of the spectrometer was carried out using an acetonitrile (CH_3CN) reference sample. Spectral data were smoothed with a Savitsky-Golay algorithm to reduce noise (2nd order, 25 point window). The spectrometer integration time was 30 seconds and each spectrum was an average of 3 acquisitions to improve consistency. Each sample of different salinity was stepped through the temperature range investigated using a temperature-controlled cuvette holder (QNW QPod2e), with a waiting time of several minutes allowed after reaching each set point to enable the water sample to reach thermal equilibrium. The reference temperature was measured using the temperature probe within the QPod2e, which has a specified accuracy of $\pm 0.15\text{ }^{\circ}\text{C}$, slightly better than the one used in [8] which had an accuracy of $\pm 0.2\text{ }^{\circ}\text{C}$. The experimental configuration is shown in Fig. 1.

Unpolarized Raman spectra were recorded for 36 combinations of temperature and salinity, resulting in a set of 108 spectra. Table 1 shows the set of temperature and salinity levels for which Raman spectra were acquired, together with the measured conductivity values used for salinity calculations. The temperature and salinity ranges cover a significant portion of the natural water conditions encountered in estuarine and coastal waters.

Table 1. **Temperature, conductivity and calculated salinity**

Temperature ($^{\circ}\text{C}$)	Conductivity (mS/cm)	Salinity (PSU)
13.0 ± 0.1	10.0 ± 0.4	5.6 ± 0.3
17.0 ± 0.1	17.0 ± 0.4	10.0 ± 0.3
21.0 ± 0.1	24.1 ± 2.0	14.6 ± 1.3
25.0 ± 0.1	32.0 ± 2	19.9 ± 1.4
29.0 ± 0.1	39.6 ± 2	25.2 ± 1.5
33.0 ± 0.1	49.6 ± 2	32.4 ± 1.5

Spectra were analyzed using both Matlab R2014b (The Mathworks) and The Unscrambler

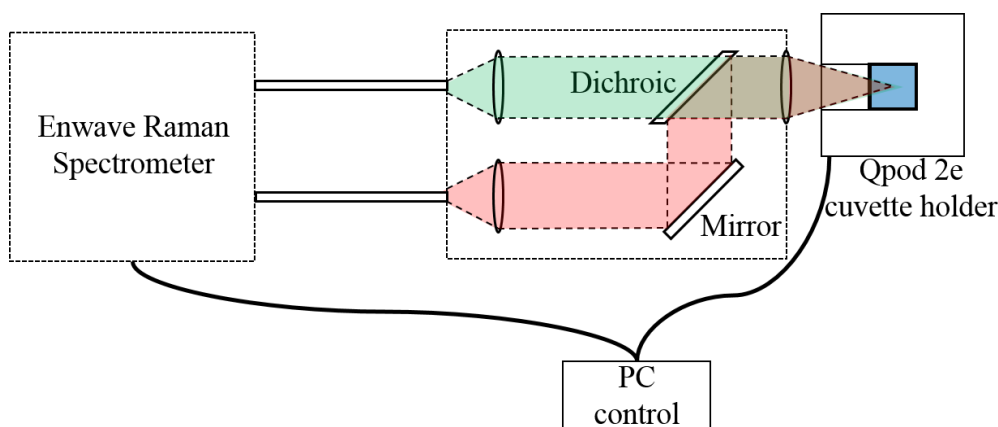


Fig. 1. Experimental setup for collection of Raman spectra.

10.2 (CAMO Software), a multivariate data analysis package. Principal Component Analysis (PCA) was employed to examine the variance of the spectral data, and then partial least squares regression (PLS-R) with full cross-validation was applied to correlate this variance with reference temperature and salinity values.

3. Raman spectra showing dependence on temperature and salinity

Unpolarized Raman spectra for water from Rose Bay are shown in Fig. 2. Figure 2 (top) shows spectra corresponding to six different temperature levels, for the case of a fixed salinity (15 PSU), while Fig. 2 (bottom) shows spectra for six different salinity levels at a fixed temperature (25 °C). The vertical axes of plotted spectra are given in terms of signal counts registered by the spectrometer (more specifically, these correspond to the CCD counts corrected for grating and spectral response), but have not otherwise been normalized or baseline corrected.

Figure 2 (top) shows a spectral response to temperature that is highly similar to the pure water case reported in [8], with an isosbestic point observed at $\sim 3410 \text{ cm}^{-1}$. In Fig. 2 (bottom), isosbestic points are observed at $\sim 3080 \text{ cm}^{-1}$ and $\sim 3250 \text{ cm}^{-1}$ in response to changing salinity. The region between these points exhibit a reduction in intensity with increasing salinity, while above $\sim 3250 \text{ cm}^{-1}$ intensity increases with increasing salinity. The maximum intensity variation with salinity is at 3410 cm^{-1} , close to the peak maxima.

Examination of Fig. 2 shows a spectral region centered around 3410 cm^{-1} where there is relatively strong dependence on salinity, but minimal dependence on temperature. Similarly, there is a spectral region centered around 3250 cm^{-1} where there is strong dependence on temperature but minimal dependence on salinity. Given these observations, it is intuitively reasonable to expect that it may be possible to simultaneously extract information concerning both temperature and salinity from Raman spectra.

4. Analysis of Raman spectra for temperature prediction

Here we consider the accuracy with which temperature can be determined from the Raman spectra in Fig. 2, where the salinity was 32.4 PSU. To do this, we followed the methods described in [8], which addressed temperature determination in pure (laboratory) water. Matlab was used to perform a least squares linear regression of the measured two-color ratio against reference temperature for each wavenumber pair:

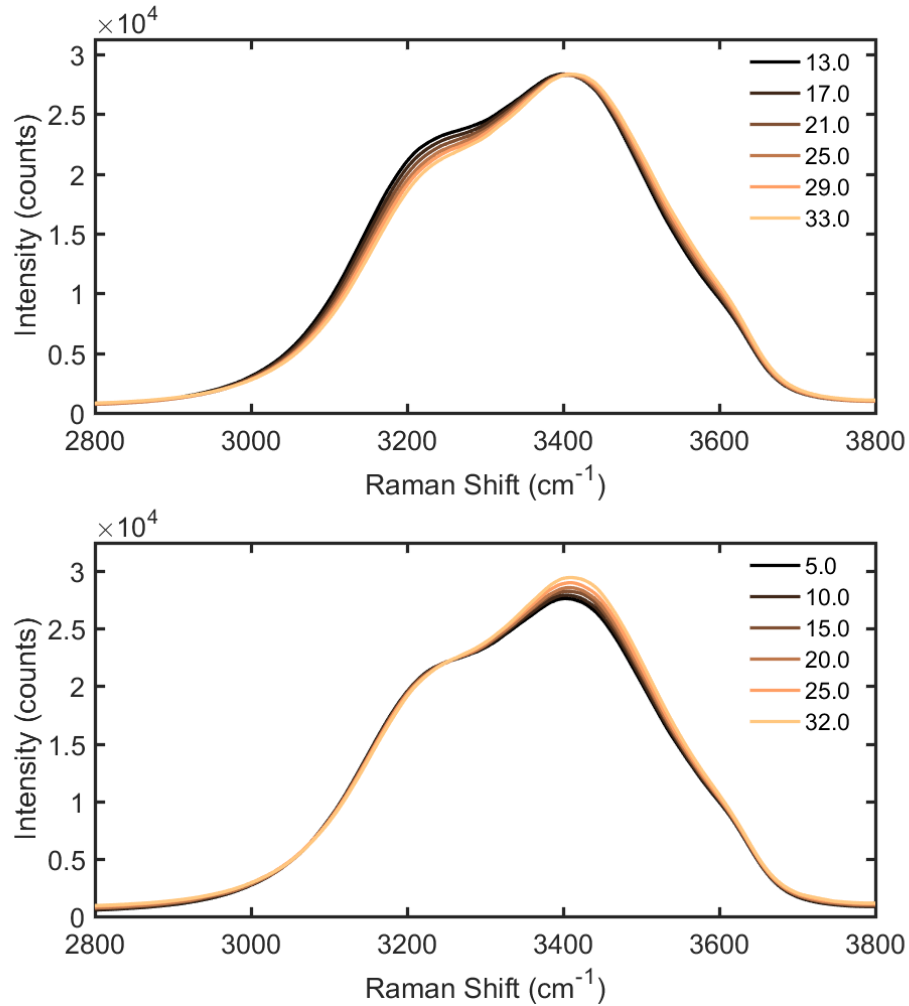


Fig. 2. (top) Raman spectra with changing temperature and fixed salinity (15 PSU). (bottom) changing salinity and fixed temperature (25 °C).

$$\text{Two-color ratio} = a \times T + b \quad (1)$$

The regression coefficients a and b were then used to build a simple predictive model for temperature, and an RMS temperature error was calculated for each wavenumber pair. We note that the accuracies achieved are a function of both the inherent temperature sensitivity of the Raman spectra, and the signal-to-noise ratio of the recorded spectra. The analysis for single wavenumber pairs, which are separated by data intervals of 0.2 cm^{-1} , is useful in identifying the "best possible" scenario for temperature accuracy. This may be useful for applications where the full Raman spectra are collected; however, in this paper we are interested in developing multi-channel instrumentation for remote-sensing which does not require the collection of full Raman spectra. Accordingly, we now simulate the case of spectral channels of width 200 cm^{-1} , which we identified in [8] as being a reasonable trade-off between temperature sensitivity and signal intensity.

Figure 3 shows a map of the RMS temperature error, computed for a wide range of band

center positions. A regions with RMS temperature error that is consistently below ± 0.2 °C is evident, as indicated by the contour line. Encouragingly, this accuracy obtained for a natural Sydney Harbour water sample, is similar to the accuracy reported for reverse-osmosis water [8].

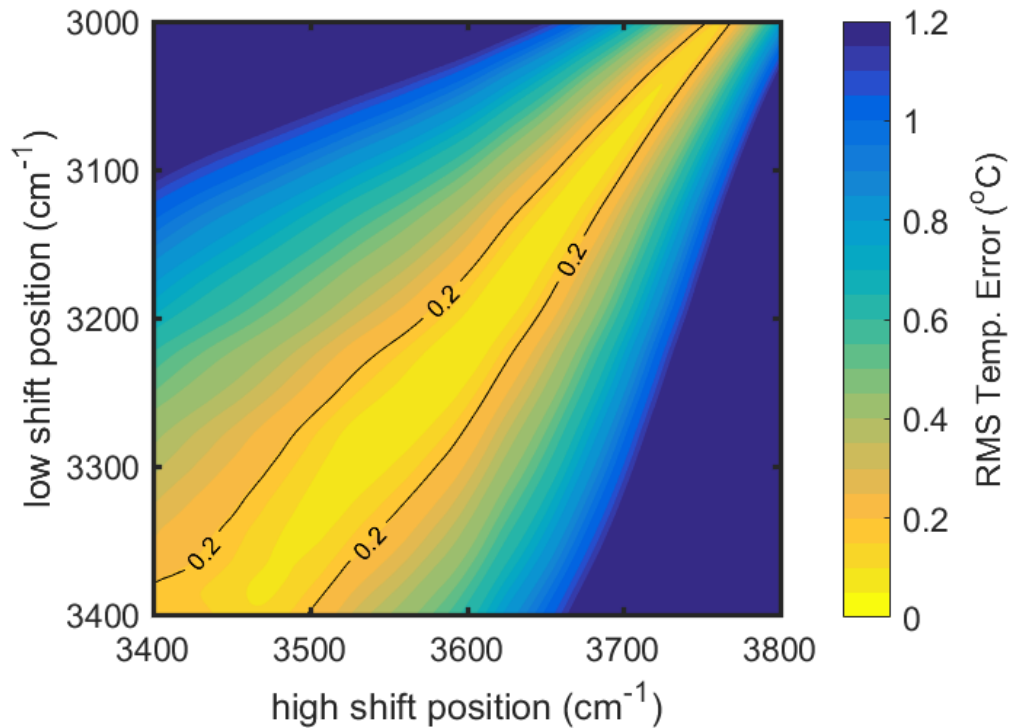


Fig. 3. Raman spectral analysis of an undiluted (32.4 PSU) Rose Bay water sample, showing RMS temperature error based on a ratio of two integrated spectral bands with 200 cm^{-1} widths. The axes represent the center position of each band.

We briefly explored the extent to which variation in the salinity of a sample had an effect on the accuracy with which temperature could be predicted. By collectively analyzing pairs of temperature-dependent spectra for which the salinity differed by 7 PSU, we found the RMS temperature error was increased to around ± 0.7 °C. Such a salinity variation includes the range over which local variations in salinity are most likely to occur.

5. Analysis of Raman spectra for salinity prediction

In this section, we explore the accuracy with which salinity can be determined from the salinity-dependent Raman spectra in Fig. 2 (bottom) where the temperature was 25 °C. The method is analogous to that in Section 4, again with spectral channels of 200 cm^{-1} width. A least squares regression of the measured two-color ratio against reference salinity was computed and the regression coefficients used to determine an RMS salinity error for each combination of spectral channels.

Figure 4 shows a map of the RMS salinity error, and it can be seen that the RMS salinity error is consistently below ± 0.6 PSU and can be as low as 0.4 PSU. We note that the RMS salinity error is well below the uncertainty calculated for reference salinity.

We examined the extent to which temperature variation had an effect on the accuracy with which salinity could be predicted. We did this by collectively analyzing two sets of salinity-

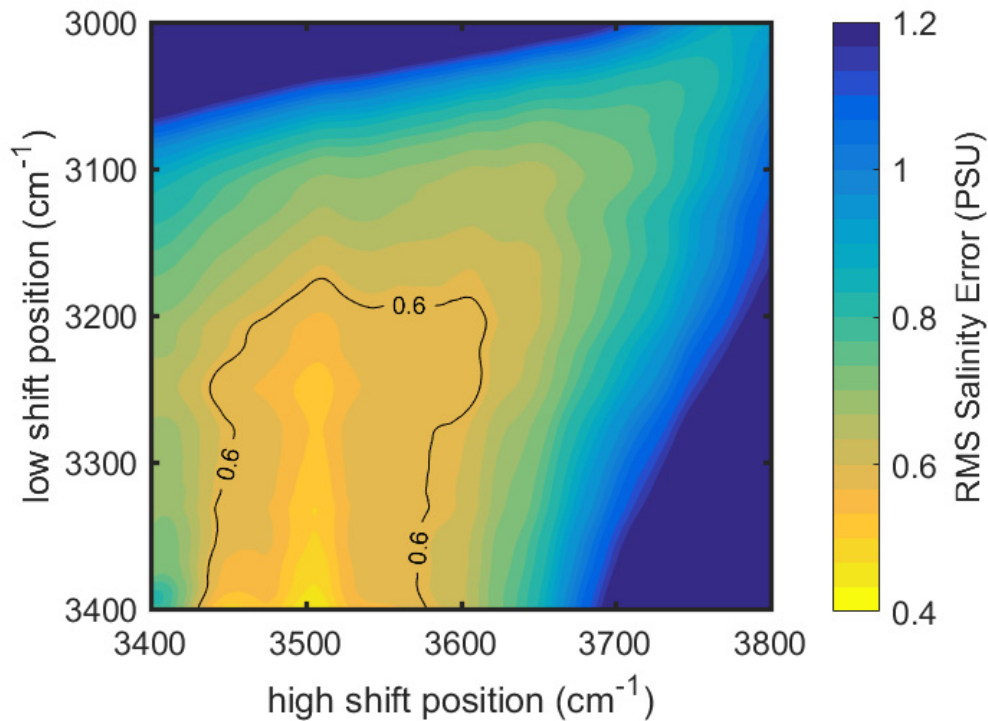


Fig. 4. Raman spectral analysis of a Rose Bay water sample at 25 °C, showing RMS salinity error based on a ratio of two integrated spectral bands with 200 cm^{-1} widths. The axes represent the center position of each band.

dependent spectra for which the temperature differed by 4 °C, and assume that this range is indicative of most local variations. For this scenario, the salinity accuracy was reduced to ± 0.6 PSU.

6. Simultaneous determination of temperature and salinity

As noted in Section 3, there are spectral regions evident in Fig. 2 where there is dependence upon either temperature or salinity. In this section, we analyze the thirty-six unpolarized stretching band spectra that were obtained for six values of temperature and six values of salinity. Partial least squares regression (PLS-R) [12] was used to explore the relationship between the spectral data and reference temperature and salinity values, and, to generate a model for estimation of these parameters. PLS-R is a multivariate data analysis method which effectively defines new axes based on the maximum variance in a set of data (spectral data in this case), making it easier to interpret behavior based on multiple parameters. Only variance in the spectra which is consistent with the changes in the reference parameter values for temperature and salinity is taken into account. The PLS-R loadings and scores plots are shown in Fig. 5.

The loadings plot (Fig. 5 (top)) displays a looping curve of points which correspond to the OH stretching band spectra between 2800 cm^{-1} and 3800 cm^{-1} . These points represent the changes in signal intensity which correspond with changing temperature and salinity, as a function of the first two factors. The regions for which greater salinity and temperature influence are observed are positioned further from the origin, and some of the data points have been labeled for clarity. The pointed section of this curve (upper-left) represents the response around 3180 cm^{-1} , where

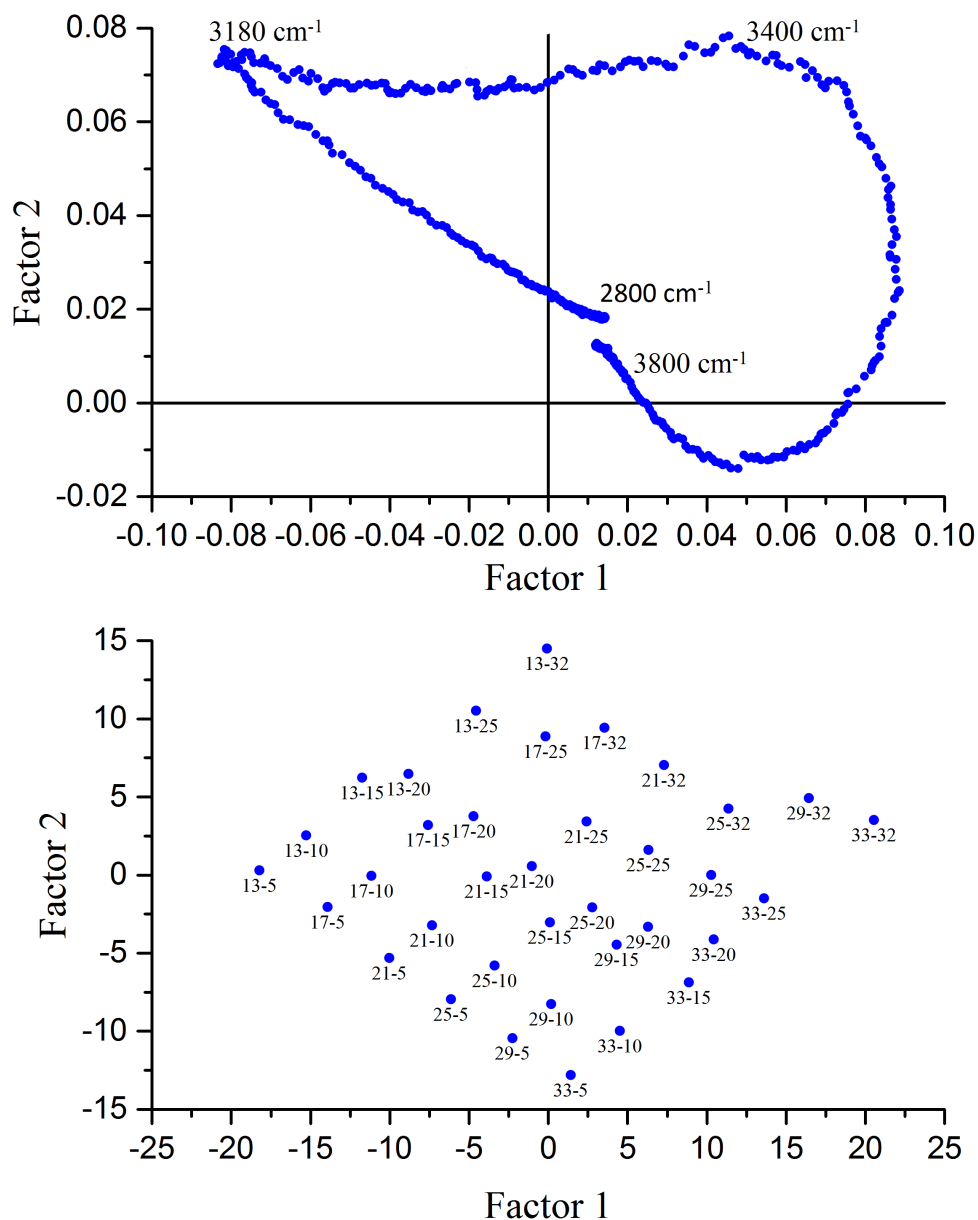


Fig. 5. PLS-R (top) loadings and (bottom) scores plots representing the behavior of the unpolarized OH stretching band ($2800\text{--}3800\text{ cm}^{-1}$). Each data point in the scores plot represents a Raman spectrum, and these are labeled with the temperature and salinity values in the following manner: "temperature-salinity".

both salinity and temperature affect the spectra in similar ways (signal intensity decreases in response to increases in both temperature and salinity). The cluster of points near the origin corresponds to spectral regions where temperature and salinity have minimal influence, and the offset of the end points of the spectral data with respect to the origin reflects the changing

baseline with temperature and salinity.

The scores plot (Fig. 5 (bottom)) depicts the variation between the spectra (represented as individual points) as a function of the first two factors. Together these first two components account for 99.9% of the variation between the Raman spectra, with 66% of variation explained by Factor 1 and 33% explained by Factor 2. Clear and systematic distinction between the spectra is evident. It is apparent that the distribution of spectra with temperature was more regular than the distribution with respect to salinity. Factor 1 shows positive correlation with both salinity and temperature, while Factor 2 shows positive correlation with salinity and negative correlation with temperature. Using two factors, the model depicted in Fig. 5 produced validation RMSE values for temperature and salinity of ± 0.6 °C and ± 1.2 PSU respectively over the temperature and salinity ranges covered. There are regions in the spectra which provide relatively little information concerning either temperature or salinity; this is apparent from Fig. 2, as well as Fig. 5 (top).

Accordingly further analysis was conducted in which these regions were removed, in order to reduce the range of spectral data required while still retaining temperature and salinity information. A set of three spectral bands, each having a spectral bandwidth of around 100 cm^{-1} were selected that could in principle be acquired using a three channel optical system. Primarily these are the regions which are strongly influenced by either temperature or salinity.

Figure 6 shows the loadings and scores plots for the three spectral band PLS-R model. This model produced validation RMSE values for temperature and salinity of ± 0.7 °C and ± 1.3 PSU respectively when using two factors. This is reasonably close to the values for the whole spectra model presented in Fig. 5, suggesting that this limited set of data retains sufficient information to make reasonable measurements of both parameters.

For a practical remote sensing application, the three spectral bands would be defined by optical filters and the integrated Raman signal would be detected with a sensitive photodetector. Such a three-channel setup was modeled by summing each band shown in Fig. 6, yielding a scores plot highly similar to that in Fig. 6 (bottom). Validation RMSE values were obtained for temperature and salinity of ± 0.7 °C and ± 1.4 PSU respectively using two factors. On the basis of this integrated model, we propose a simple optical system in which three spectral bands could be acquired in order to simultaneously extract temperature and salinity values, and this is depicted in Fig. 7.

The excitation laser, assumed here to have a wavelength of 532 nm, is directed into the water sample via dichroic mirror (DM). Raman scattered radiation in the red spectral region passes through DM and a long pass filter (LP) for rejection of scattered or reflected light at 532 nm. It is then directed by two beam-splitters (BS) to three photomultipliers (PMT), each fitted with a band-pass filter (BP1, BP2, BP3) to select appropriate spectral bands (approximately 3150 to 3280, 3370 to 3466 and 3500 to 3600 cm^{-1}). A pulsed excitation laser in combination with LIDAR techniques would enable depth-resolved measurements of temperature and salinity.

7. Discussion

The temperature-dependent and salinity-dependent Raman spectra obtained for a natural water sample and presented in Fig. 2 are of very high quality, and the relatively-high signal to noise ratio is an important contributing factor enabling us to extract information about temperature and salinity with reasonable accuracy. Considering the case of 200 cm^{-1} spectral bands, which provide a good compromise between both good sensitivity to temperature (or salinity) and good signal intensity, we have shown that temperature and salinity can be predicted with RMS errors below ± 0.2 °C and ± 0.4 PSU in the case where there is no variation in the other.

PCA and PLS-R offer means by which the variance within the spectral data can be visualized, in a way that has not previously been considered. These tools were used to quantitatively explore which portions of the spectra contained the most "information" about temperature and salinity,

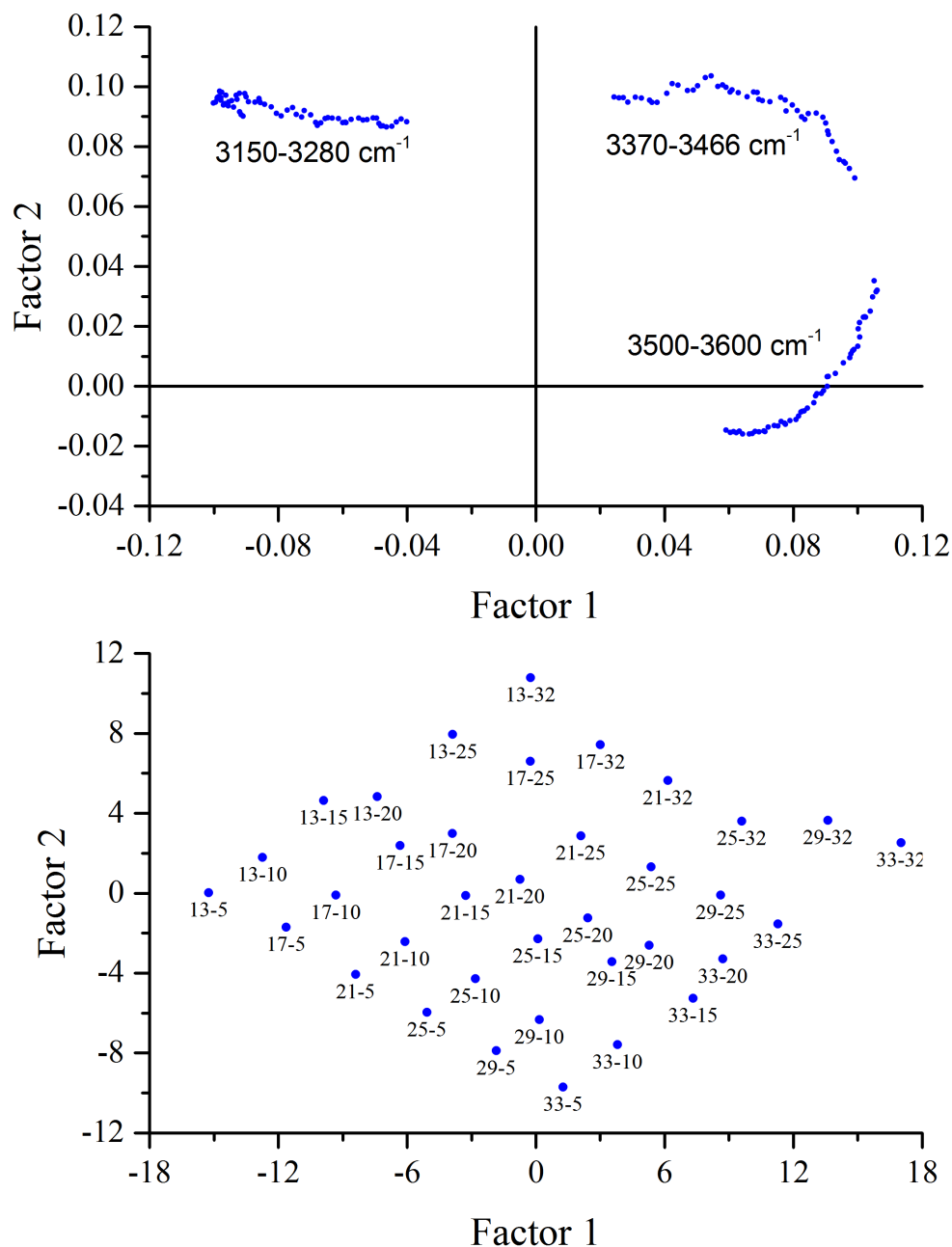


Fig. 6. PLS-R (top) loadings and (bottom) scores plots representing the behavior of three spectral regions from the OH band with unpolarized detection. Each data point in the scores plot represents a Raman spectrum, and these are labeled with the temperature and salinity values in the following manner: "temperature-salinity".

leading to the identification of three spectral regions which correlate strongly with variation of one or both parameters. When variations in both temperature and salinity are considered, we

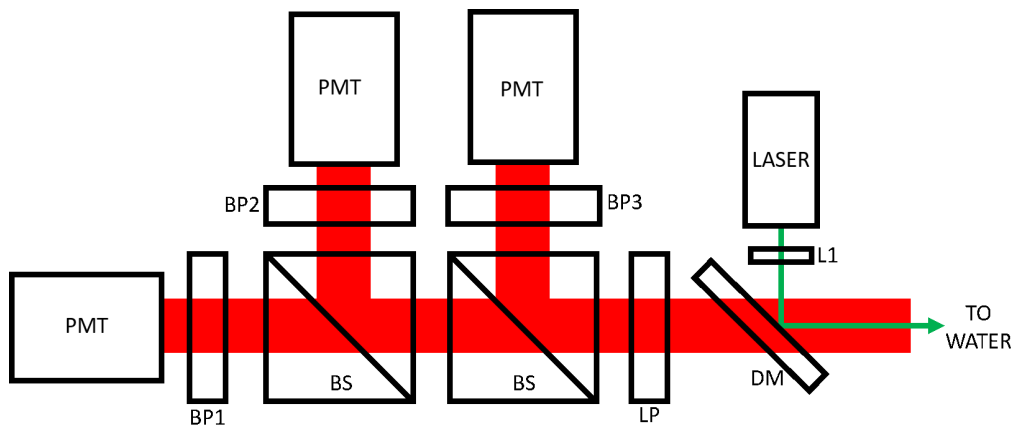


Fig. 7. A three-channel Raman detection system for simultaneous collection of temperature and salinity data.

have shown it is possible to determine both temperature and salinity from unpolarized Raman spectra of water samples with RMSE values of ± 0.7 °C and ± 1.3 PSU. Here 100 cm^{-1} spectral bands were necessary to avoid overlapping bands. We note that the natural water sample investigated here is relatively clean, with low levels of organics. Further work will be required to determine the extent to which higher levels of organic content, which could lead to a fluorescence spectrum being overlaid on the Raman spectra, impact on determination of temperature and salinity in a wider range of water samples.

The accuracy with which temperature was predicted here, in the absence of salinity variation, is similar to what was reported in [7, 8] for laboratory water, and compares favorably with what has been reported by other groups for natural water samples [5, 10, 13]. The determination of salinity using Raman spectroscopy has been investigated less-widely, and accordingly it is more difficult to draw comparisons. The authors of [1, 10] have applied neural networking methods to simultaneously determine temperature and salinity from the shape of the Raman band. They reported mean absolute errors of 0.5 °C and 0.7 PSU in NaCl solutions, and errors of 1.1 °C and 1.5 PSU in natural waters that included dissolved organic matter. These errors are broadly similar to those reported in this paper, considering the differences in water samples, and possible differences in the way that errors were determined. The essential difference between our two approaches is that to solve the two parameter inverse problem, the full Raman band spectra is required, and this precludes the retrieval of depth-resolved temperature information.

We note that several papers [14–17] have investigated the use of Brillouin scattering to determine temperature, with one of these proposing to deduce both temperature and salinity from the measured Brillouin shift [17]. Here, the principle is that temperature and salinity both affect the speed of sound, and it is the speed of sound that determines the measured Brillouin shift. While Brillouin scattering has been used to infer temperature, it is usually necessary to make an assumption about the value of salinity [14, 15]. However based on Brillouin scattering theory, [17] presents simulations to support his proposal to simultaneously extract temperature and salinity from the Brillouin signal. In our view, there are complexities in the use of Brillouin scattering that are not present in Raman spectroscopy. These include a laser source having narrow line-width and a means for measuring the frequency shift between excitation and Brillouin signals, which is typically around 7-8 GHz in water. It would however be interesting to explore how Brillouin and Raman scattering might be used in concert to obtain enhanced information about the water column.

On the basis of the multivariate analysis presented here, we have proposed a simple three-

channel spectrometer that could in principle be used for depth-resolved measurements of temperature and salinity. The specifications for narrow band-pass filters are quite stringent, but these are within the scope of commercially-available custom-designed filters. In the future, we will evaluate the performance of such a spectrometer in combination with a short-pulse excitation laser for depth-resolved measurement of temperature and salinity.

8. Conclusion

We have applied multivariate analysis methods to quantitatively visualize the variance in the Raman spectra of a natural water sample as a function of temperature and salinity. Based on the analysis, we have developed straightforward methods for extracting information about temperature and salinity from this sample, both individually and simultaneously, and presented the corresponding RMS temperature and salinity errors. Finally, we have proposed a three-channel spectrometer for the simultaneous determination of temperature and salinity; simulations for our particular water sample predict that temperature and salinity could be extracted with accuracies of ± 0.7 °C and ± 1.4 PSU.

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