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ARCoptix Switzerland

Application note

Measurement of concentration of CO_2 in water using integrated Rocket ATR spectrometer

Introduction

The Arcoptix OEM-ATR-20-12 spectrometer is an ATR (attenuated total reflection) version of the Arcoptix very successful range of spectrometers, adapted for measurements of liquids. This Application note is documenting the use of this spectrometer for measurement of diluted CO2 in water.

Method

A saturated solution of CO2 in water has been prepared out of degassed deionized water and technical CO2 by supersaturating the water at increased pressure in the CO2 atmosphere. The supersaturated solution was then left to come to equilibrium at the atmospheric pressure, still under the atmosphere of CO2 in the altitude of 380 meters and QNH 1002 hPa. According to the published nomograms the initial concentration at 30 °C was at 450 ppm with the uncertainty of 10%. The solution was then sequentially diluted following a geometrical sequence with a factor of ½. The final concentration in the sequence of measurements is in the range of 7 ppm.

Procedure:

(1) The background spectrum was measured with degassed deionized water on the crystal, integrating individual 256 spectra with the resolution of 2 cm^{-1}.
(2) The ATR crystal was then dried, and the sample was deposited using a micro-pipet.
(3) The sample was left to stabilize for 1 minute and a spectrum integrating 256 spectra was taken in absorbance mode.
(4) The recorded spectra were then investigated at 2344 cm^{-1}, where the maximum of the diluted CO2 is located.
(5) Reproducibility was tested using two subsequent measurements at 14 ppm, the noise equivalent concentration has been evaluated and the theoretical maximum available concentration has been determined as well as the sensitivity of the method.

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Results

(1) The detail of the absorption peak corresponding to the dissolved CO2 for 2344 wavenumbers plotted for the variety of the concentrations is shown below.

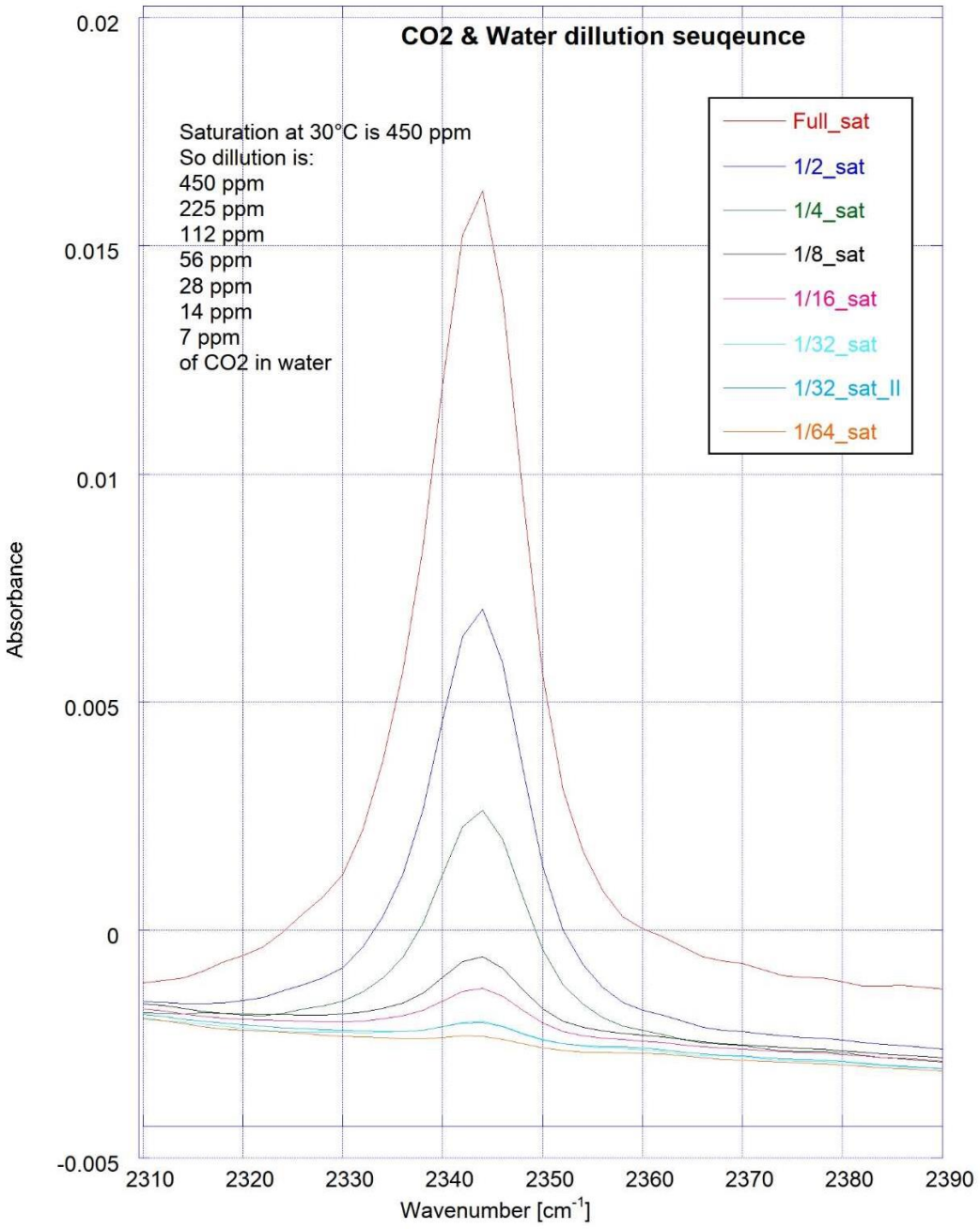

Figure 1 – CO2 in water for various concentrations the dilution follows a geometric sequence with a factor of 0.5.

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(2) The reproducibility has been tested for the concentration of 14 ppm by two consecutive measurments. The plot is shown below. The noise on the level of 2.2e-5 of absorbance has been detected.

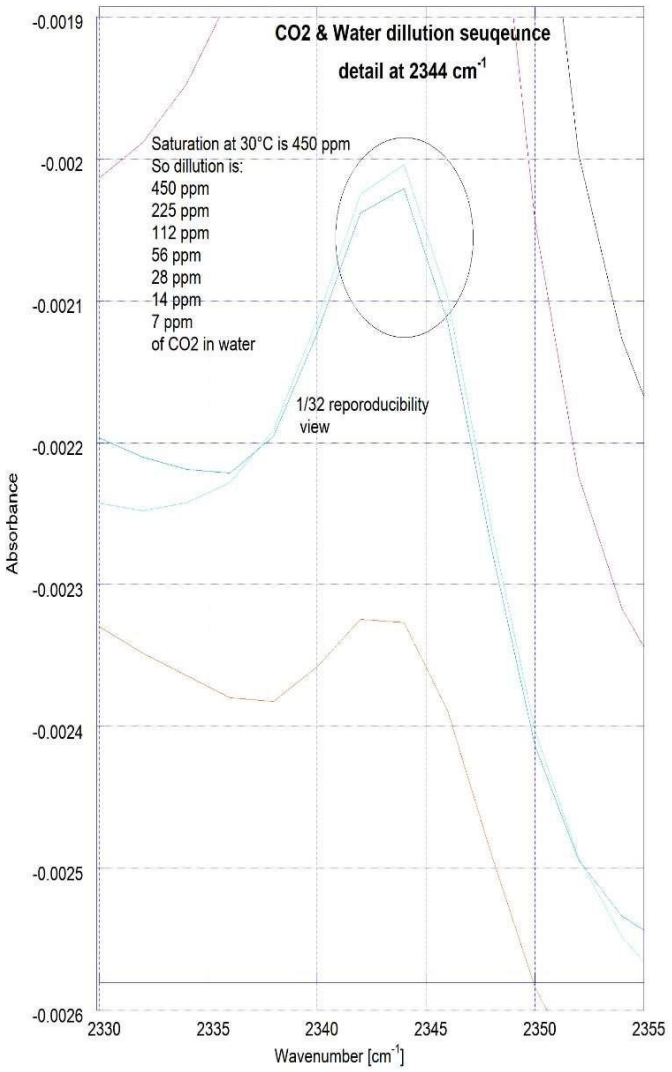

Figure 2 – Reproducibility test performed at 14 ppm of the concentration.

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(3) The sensitivity evaluation. For simplicity only the maxiam of the asorbance signal with respect to the concentration at the 2344 wavenumbers have been plotted. With this respect the sensitivity of this method in the level of 3.70 e-05 of absorbance per ppm have been detected in the vicinity of the zero point (four lowest points have been line-fitted, and the slope has been evaluated). According to this the noise equivalent concentration of 0.605 ppm have been determined (the LOD and LOQ determination would require more data in the dataset to be evaluated).

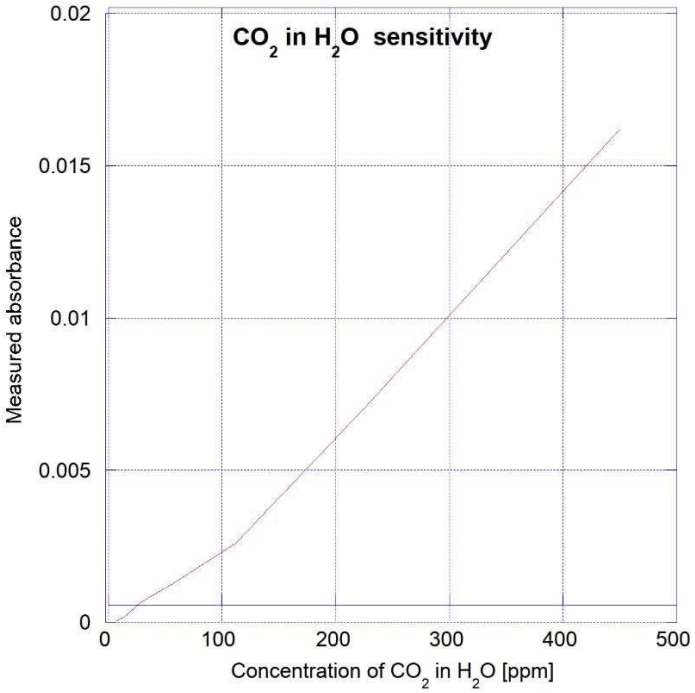

Figure 3- >Evaluation of the sensitivity of OEM- ATR-20-12 model for binary mixture of Carbon dioxide in water.

Conclusion.

The OEM-ATR-20-12 has been evaluated as a suitable tool for measurements of the diluted Carbon dioxide in water on the ppm level. Further – more sophisticated evaluation is to be performed to quantify the performance and to narrow down the margins of the precision.

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