SOCRATES GV Ice Spectrometer measurements

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1.0 Data Set Overview

These measurements were part of the Southern Ocean Clouds Radiation Transport Aerosol Transport Experimental Study (SOCRATES). The main objective of the SOCRATES experiment is to improve our understanding of aerosol-cloud interactions with respect to the major synoptic meteorological conditions in the Southern Ocean (SO) to reduce the uncertainties related to aerosols, clouds and their feedbacks in our climate models. Specifically, PI DeMott's group deployed instrumentation for measuring ice nucleating particles (INPs) and bio-aerosols on multiple platforms. This archive relates to the Colorado State University Ice Spectrometer (IS) instrument that utilized filters collected onboard the NSF/NCAR HIAPER G-V during SOCRATES in order to measure the immersion freezing temperature spectra of ambient particles. The IS was used to measure INP number concentrations during approximately level-leg transects in the marine boundary layer (MBL) or above clouds, to determine their relation to ocean sources and long-range transport of aerosol and cloud microphysical properties in the Southern Ocean region. Flights were based from Hobart, Tasmania. The time period covered is January 15 to February 24, 2018. A total of 15 research flights were flown with the CFDC instrument operational at latitudes between -42.5 and -62.5 degrees and longitudes 134 to 163 degrees, and altitudes within the lower 6 km of the Earth's atmosphere.

2.0 Instrument Description:

The Colorado State University Ice Spectrometer (IS) emanates from the developments of Hill et al. (2014; 2016) and is described in the approximate present form by Hiranuma et al. (2015) and DeMott et al. (2018). Immersion freezing temperature spectra are obtained in the IS following dispensing 24 or 32 aliquots of 30 to 60 µL suspensions of aerosols into sterile wells that are isolated in a cooled device that is purged by ultra-clean nitrogen gas. Temperature is lowered at 0.33°C min^{-1} and frozen wells are counted at 0.2-1°C degree intervals to a limit of approximately -28°C. Cumulative numbers of INPs mL^{-1} of suspension are estimated on the basis of Vali (1971) using,

$$c_{IN}(T) = -\frac{\ln\left(f_{unfrozen}(T)\right)}{V_{drop}} \quad (1)$$

where $c_{IN}(T)$ is the concentration of INPs per unit volume of water (m^{-3}), $f_{unfrozen}$ is the fraction of unfrozen drops at T, and V_{drop} is the population-median drop volume. Volumetric INP concentrations in air ($C_{INP}(T)$) are calculated via,

$$c_{INP}(T) = \frac{c_{IN}(T) \cdot f \cdot V_{imp}}{V_a} \quad (2)$$

where V_{imp} is the total volume rinsed from a collection filter), f accounts for any dilution of the suspension (f = 1 for undiluted), and V_a is the air volume collected into liquid. Filter blanks are collected and processed in a similar manner as aerosol samples to obtain a mean background INP spectrum.

Filter samples were obtained on the GV using 47-mm diameter in-line aluminum filter holders fitted with a 0.2 µm diameter pore Nuclepore polycarbonate membranes. These were located within the CFDC instrument rack. Sampling was from the HIMEL inlet (same as used for the CFDC) at all times. After flights, filters were transferred using clean, protocol and stored frozen at -20°C before shipping frozen to CSU. For re-suspension of particles, filters are placed in sterile 50 mL Falcon polypropylene tubes), 6-10 mL of suspension solution is added and particles are re-suspended by tumbling end-over-end at 60 cycles min^{-1} for 20 min. Ultra-filtered water used in experiments typically contain 1.6 INPs mL^{-1} at -25°C, and this sets typical lower detection limits. Correction is then applied for the number of INPs processed from rinsed filter blanks that were carried onto the GV during several flights.

A filter rinse produces sufficient volume for standard processing as described above, and alternate treatments prior to freezing tests to give inference to INP compositions. These treatments include thermal exposure of suspensions at 95°C for 30 minutes to destabilize biological ice nucleating proteins (typically destroying their activity as INPs while not affecting inorganic INPs) or digestion of all organic carbon through application of hydrogen peroxide (Suski et al., 2018). The latter test distinguishes total organic versus inorganic INPs. As it is uncertain if the particle number and mass are sufficient for application of the latter test, the initial archive uses a “heat_treat_flag” only, to reflect that it is likely that the heat treatment will be the only type applied at the time of final archival. If the peroxide treatment is performed, the header will be revised to add the additional treatment flag.

3.0 Data Collection and Processing:

IS filter collections represent integrated volumes collected over extended times of sampling at standard flow rates that varied by altitude from several to 15 lpm. Oftentimes, collections included multiple passes at similar altitudes, but at different locations considered representative of the MBL or above-cloud region for target cloud systems. This made the IS data for SOCRATES the most complicated for archival of any yet assembled, requiring a long list of secondary variable information.

The primary data are INP concentrations as a function of temperature, and the 95% negative and positive confidence intervals for these, and a flag for special sample processing as described in the previous section. Binomial sampling confidence intervals (95%) are derived for all data using the formula recommended by Agresti and Coull (1998):

$$\mathrm{CI}_{95\%} = \left(\hat{p} + \frac{1.96^2}{2n} \pm 1.96\sqrt{\left[\hat{p}(1-\hat{p}) + {1.96^2}/{4n}\right]/n}\right) / \left(1 + {1.96^2}/{n}\right) \quad (3)$$

where $\hat{p}$ is the proportion of droplets frozen and *n* is the total number of droplets. Using this formula, for a single well frozen out of 32 aliquots the $\mathrm{CI}_{95\%}$ ranges from 18% to 540% of the estimated INP concentration, while for 16/32 wells frozen it is 68-132% of the INP concentration.

4.0 Data Format:

IS data are reported in non-standard ICARTT format to account for the fact that filters were often integrated over multiple passes at different locations in order to increase sample volumes representative of the MBL or the above-cloud region. The primary variables and units are given in the data file header, but are repeated here. Processed data appear as arrays, led by a list of secondary time, location and altitude variables. These lines, one for each filter collected on a flight, begin with:

start_time, fraction of day in UTC, Time_Start

and include the following information,

start_date_day_1, UTC date
start_date_month_1, UTC month
start_date_year_1, UTC year
stop_time_1, fraction of day in UTC
stop_date_day_1, UTC date
stop_date_month_1, UTC month
stop_date_year_1, UTC year
start_Lat_1, degrees decimal, Latitude
start_Lon_1, degrees decimal, Longitude
end_Lat_1, degrees decimal, Latitude
end_Lon_1, degrees decimal, Longitude
Altitude_1, m, MSL

Total_volume_filtered_1, liters
start_time_2, fraction of day in UTC
…

Each line extends to reflect sampling during up to 5 different collection periods for a single IS filter. INP data then follow for each filter as arrays that are led by,

TempC[],degC, Temperature_array, degrees Celcius

and also include,

N_INP[], #/liter, INP_Ambient_NumDensity_array
CL_INP_LOWER[], #/std-liter, INP_95%_Conf_interval_lower_array
CL_INP_UPPER[], #/std-liter, INP_95%_Conf_interval_upper_array
heat_treat_flag[], none, heat_treat_flag_array ; {0 = none, 1 = 95C}

All INP concentrations are at STP conditions (0C, 1013.5 mb), although the variable names do not include the STP designation.

The file names archived as "preliminary" are:
IS_SOCRATES_GV_RF01_20180115_R1.ict
IS_SOCRATES_GV_RF02_20180119_R1.ict
IS_SOCRATES_GV_RF03_20180122_R1.ict
IS_SOCRATES_GV_RF04_20180123_R1.ict
IS_SOCRATES_GV_RF05_20180125_R1.ict
IS_SOCRATES_GV_RF06_20180128_R1.ict
IS_SOCRATES_GV_RF07_20180131_R1.ict
IS_SOCRATES_GV_RF08_20180203_R1.ict
IS_SOCRATES_GV_RF09_20180204_R1.ict
IS_SOCRATES_GV_RF10_20180207_R1.ict
IS_SOCRATES_GV_RF11_20180217_R1.ict
IS_SOCRATES_GV_RF12_20180218_R1.ict
IS_SOCRATES_GV_RF13_20180219_R1.ict
IS_SOCRATES_GV_RF14_20180221_R1.ict
IS_SOCRATES_GV_RF15_20180224_R1.ict

Final file versions will have a different version extension. Missing or erroneous values are reported as -9999. For example, after background (blank) correction, some IS INP concentrations became slightly negative, meaning that they were not resolvable at greater than blank INP concentrations. The -9999 values also appear in the lead in time/location line if less than five sample periods were used.

5.0 Data Remarks

The complex and integrated nature of the IS samples has been discussed above. Due to the extremely low INP concentrations and the limited volumes of samples compared to ship or fixed-site collections that typically last for 24 hours or more, background corrections are significant for this data set. While CI values are provided as for all past archived IS data, a flag to indicate the statistical significance of data has not been added to this first (preliminary) archive. We are evaluating an appropriate statistical test at this time. This is especially relevant to considering the significance of the rare first well or two freezing in advance of the majority of wells. For this reason, we must emphasize that one should probably not focus or yet apply any significance to the rare activity found at temperatures above -15°C (and perhaps even colder) in some samples.

6.0 References

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