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Supplement of

Estimation of reactive inorganic iodine fluxes in the Indian and Southern Ocean marine boundary layer

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Supplementary Text

1. Abbreviations used in the text:

ISOE-8	8th Indian Southern Ocean Expedition
IIOE-2	2nd International Indian Ocean Expedition
ISOE-9	9th Indian Southern Ocean Expedition
SK-333	Sagar Kanya-333 expedition in the south Indian Ocean
BoBBLE	Bay of Bengal Boundary Layer Experiments
Chl-*a*	Chlorophyll-*a*
HYSPLIT	HYbrid Single-Particle Lagrangian Integrated Trajectory (HYSPLIT) model (Rolph et al., 2017; Stein et al., 2015)
DSCD(s)	Differential slant column density(ies)

2. Multiple linear regression analysis

A region-specific parameterisation tool for estimating sea surface iodide concentration was developed following the (Chance et al., 2014) method. Observations for SSI concentrations from ISOE-9, SK-333 and BoBBLE were used for the multiple linear regression analysis against various atmospheric and oceanic parameters. SST data used for linear regression analysis was recorded during ISOE-9 using a bucket thermometer at an interval of 6 hours accounting for a change of approximately 1 degree in the latitudinal track of the ship and simultaneously during each seawater iodide sampling. Seawater samples collected during ISOE-9 at the same interval as the recorded SST were used for salinity retrievals using the AUTOSAL salinometer. For the SK-333 and BoBBLE expeditions most of the samples were collected from the CTD casts and some (4 data points) were underway samples in case of

BoBBLE expedition. The MLD climatological monthly mean computed from climatological monthly mean profiles of potential temperature and potential density based on three different criteria was obtained using the World Ocean Atlas (Monterey and Levitus, 1997). That being; a temperature change from the ocean surface of 0.5 degree Celsius (MLD_{pt}), a density change from the ocean surface of 0.125 (sigma units) (MLD_{pd}), and a variable density change from the ocean surface corresponding to a temperature change of 0.5 degree Celsius (MLD_{vd}) (Monterey and Levitus, 1997). All three climatological monthly mean MLD data types (MLD_{pd}, MLD_{pt}, and MLD_{vd}) were used for linear regression with measured iodide concentration. The climatological monthly mean of sea surface nitrate concentrations for ISOE-9 was also obtained from the World Ocean Atlas 2013, version 2 (Garcia et al., 2013). Chl-*a* data for ISOE-9 was obtained from pigment analysis during ISOE-9.

3. Dataset used for SSI estimation

For estimating the SSI concentrations for all campaigns (ISOE-8, IIOE-2, and ISOE-9) using parameterisation methods in Eq. (1) to (5), the oceanic parameters were obtained from the observations during individual campaigns. Missing data was substituted with available data, as in the case of IIOE-2 campaign. For this campaign, salinity data was obtained from the World Ocean Atlas 2013, version 2 (Zweng et al., 2013). Also, chl-*a* data for IIOE-2 was obtained from level 3 daily and 8-day products of Aqua MODIS satellite (NASA-GSFC, 2017). Similarly, sea surface nitrate concentrations and MLD for all the campaigns were obtained from World Ocean Atlas (Garcia et al., 2013; Monterey and Levitus, 1997).

4. Parameterisation for SSI estimation

Chance et al. (2014) developed two versions of empirical relationship for SSI estimation. The first one is given in the main text (Eq. 1). For the regional specific modification (Eq. 2 and 3), each of the oceanic parameters was obtained for the same location (SST, salinity, chl-*a*) as the measured SSI concentrations from ISOE-9, SK-333 and BoBBLE. Likewise, monthly climatological datasets were obtained for MLD and nitrate with a one-degree spatial resolution, as described in the previous section. The regression analysis for region-specific modification was initially divided in three sections – first for the all the SSI observations including the Indian Ocean and the Southern Ocean (ISOE-9, SK-333, and BoBBLE). The second only for the Southern Ocean region (ISOE-9) and lastly only the Indian Ocean region (SK-333 and BoBBLE). A list of adjusted R^2, slope, intercept and significance of all parameters for linear regression with observed iodide concentration is provided in Table S1. The third scenario resulted insignificant coefficient of determination values (R^2) for individual parameters. In this case, latitude and salinity were the only parameters that showed significant dependence on the observed SSI (Table S1). Individual parameters with significant R^2 values were used to obtain a parametric equation for SSI concentration. The first, second, and third scenario resulting in parametrisation denoted by Eq. (2), Eq. (3), and Eq. (3a) respectively are given in the main text in Table 2. A combination similar to the Chance parameterisation given in Eq. (2) gave maximum R^2 value of 0.794 (N = 128) for the Indian Ocean and the Southern Ocean region. In this equation, all parameters are significant except for salinity and nitrate concentration. Removal of any one of these insignificant parameters did not make the other significant. The coefficient for this equation (Eq. 2) also remained insignificant with high error value (22 ± 137). The combination of SST^2, latitude, nitrate and salinity resulted in a maximum $R^2 = 0.86$ (N=110) for the dependent variable [iodide] in Eq. (3). The inclusion of MLD_{pt} (with highest R^2 for MLD) increased the R^2 slightly but had a non-uniform distribution of the residuals and was thus excluded. Similarly, the addition of chl-*a* to the equation did not change the R^2 significantly, and thus chl-*a* was removed from the final equation. The Indian Ocean scenario parameterisation in Eq. (3a) obtained $R^2 = 0.325$ (N=18). All parameters (latitude, salinity) and the coefficient were insignificant with large error values as shown in Table 2. These equation datasets were tested for statistical robustness by ANOVA test using StatPlus analysis software. Both equation (2) and (3) dataset result in higher F ratio value corresponding to the critical F value from f-distribution table and p-value < 0.0001 at 0.05 significance level. Eq. (2) obtains $F = 94$ with (5, 122) degree of freedom (critical value = 2.289) and Eq. (3) obtains $F = 161$ with (4,105) degree of freedom (critical value = 2.458). However, Eq. (3a) Indian Ocean dataset provides statistically insignificant result as the F value 3.604 with (2,15) degree of freedom is lower than the critical value of 3.682 with $p = 0.053$. Thus, this parameterisation is omitted from further analysis in the study and is indicative that the sea surface iodide estimation in the Indian Ocean does not follow the Chance parameterisation technique. It is important to note that this analysis involved a small dataset (N=18) and more observational studies will be required to estimate iodide concentrations in this region. SSI concentration was also estimated using the logarithmic parameterisation by Chance et al. (2014) and it was found to be higher in comparison to the measured SSI concentration from ISOE-9. The ln[iodide] equation estimated SSI concentrations of ~500 nM in the Indian Ocean region which is very high compared to global observations of SSI in the Indian Ocean (Chance et al., 2014, Chance et al., 2019) and in comparison to the observations from SK-333 and BoBBLE for the South Indian Ocean. Therefore, we excluded the logarithmic parametrization for this study and suggest that the ln[iodide] parametrization is not adequate for SSI estimation.

5. References

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6. Figures

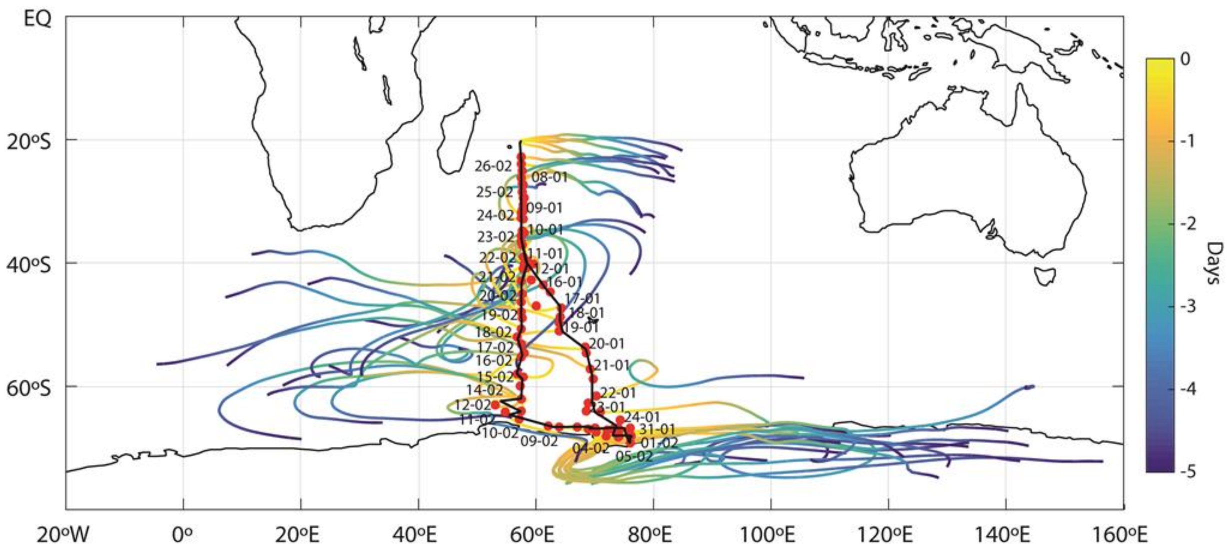

Figure S1: Map of the south Indian Ocean and the Southern Ocean showing the cruise track (black line) for the ISOE-9 campaign. Along the cruise track 5-days backward wind trajectories (HYSPLIT) of the air masses arriving the locations at noon each day of the ISOE-9 expedition. Sea surface iodide sampling locations marked in red circles along with the date of sampling.

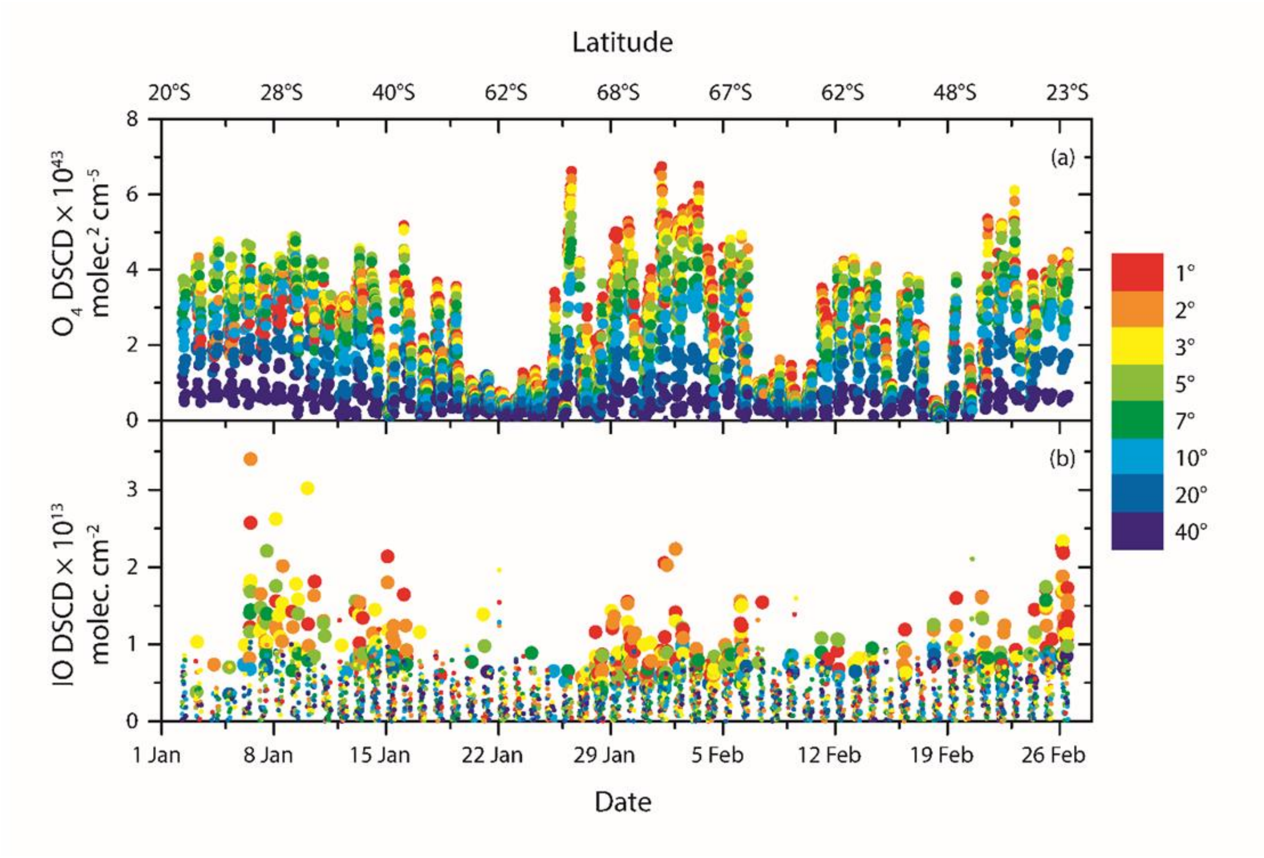

Figure S2: Timeline of the O_4 and IO DSCDs observed during the ISOE-9 expedition. The top scale indicates corresponding latitudes for the dates, and colour code represents the elevation angle (°) for each scan. Smaller circles indicate DSCDs below σ detection limit for IO and 2σ in case of O_4; bigger circles indicate DSCDs above the detection limit respectively.

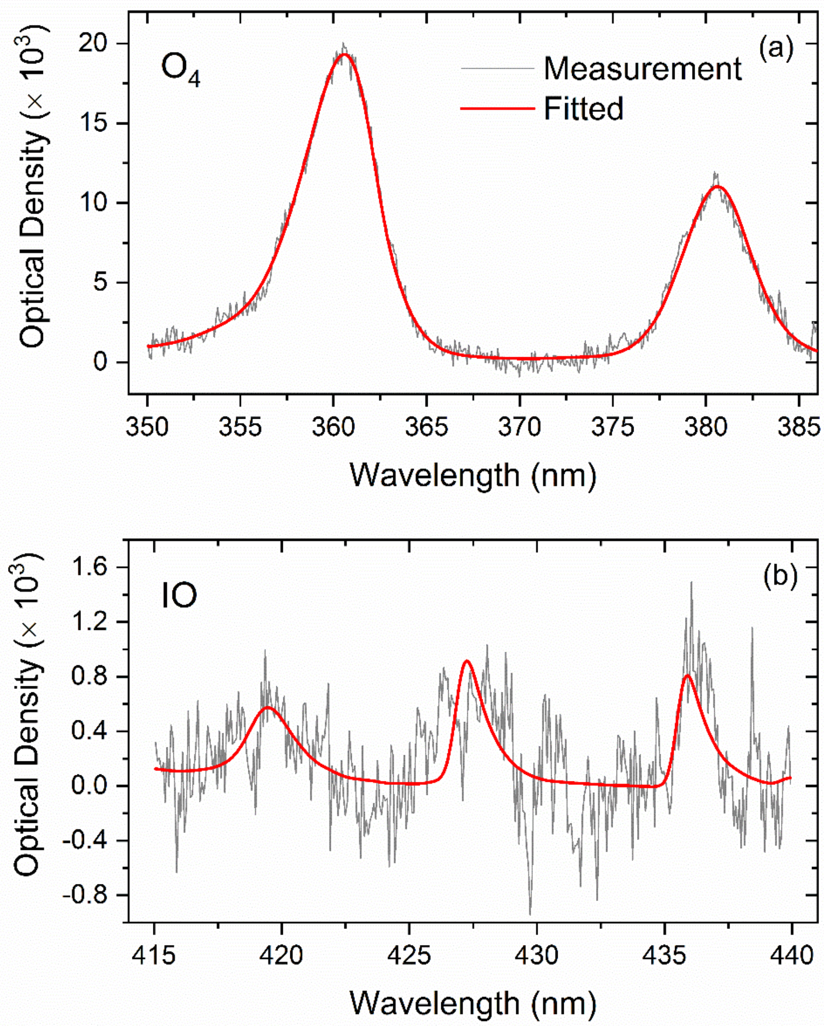

Figure S3: An example of typical spectral fit for O_4 (a) and IO (b) during the ISOE-9 expedition. These spectral fits were taken on 26 February 2017 at 15:35 (local time), for solar zenith angle 69.5° and 1° elevation angle. These fits retrieved O_4 slant column density of $(4.35\pm0.035)\times10^{43}$ molecules cm^{-2} and $(2.24\pm0.36)\times10^{13}$ molecules cm^{-2} with residual optical density (root mean square) of 3.2×10^{-4} and 5.5×10^{-4} respectively.

7. Tables

Parameter	R^2	Slope (m)	Intercept (C)	p < 5%? (p)
SST	0.64	4.26 ± 0.29	31 ± 4.77	Yes (0)
	0.62	*4.03 ± 0.304*	*32.2 ± 4.17*	*Yes (0)*
	0.07	28.8 ± 26.22	-668.85 ± 754.52	No (0.29)
1/SST (K^{-1})	0.62	-345781 ± 23910	1297 ± 83.9	Yes (0)
	0.59	*-322918 ± 25302*	*1215 ± 89.5*	*Yes (0)*
	0.07	-2616459 ± 2392959	8826 ± 7926	No (0.29)
SST^2	0.73	0.16 ± 0.0085	41.1 ± 3.6	Yes (0)
	0.79	*0.18 ± 0.01*	*39.2 ± 2.7*	*Yes (0)*
	0.07	0.51 ± 0.45	-261.9 ± 375.2	No (0.28)
NO_3	0.42	-3.24 ± 0.34	125 ± 5.7	Yes (0)
	0.39	*-2.63 ± 0.32*	*110.6 ± 5.8*	*Yes (3.06×10^{-13})*
	0.03	19.34 ± 27	153 ± 17	No (0.48)
|Latitude|	0.55	-2.1 ± 0.17	178.3 ± 8.3	Yes (0)
	0.52	*-2.43 ± 0.22*	*196.1 ± 11.7*	*Yes (0)*
	0.30	8.74 ± 3.35	108.5 ± 23.11	Yes (0.02)
Monthly MLD_{pt}	0.17	-1.1 ± 0.22	125 ± 9.2	Yes (1.2×10^{-6})
	0.08	*-0.63 ± 0.21*	*97.6 ± 9.4*	*Yes (0.003)*
	0.14	-2.69 ± 1.68	203.41 ± 30.38	No (0.13)
Monthly MLD_{vd}	0.04	-0.48 ± 0.2	98 ± 8	Yes (0.03)
	0.003	*-0.11 ± 0.19*	*75.9 ± 7.5*	*No (0.56)*
	0.16	-2.69 ± 1.55	193.52 ± 23.6	No (0.10)
Monthly MLD_{pd}	0.12	-0.67 ± 0.16	110 ± 7.8	Yes (5.2×10^{-5})
	0.05	*-0.35 ± 0.15*	*87.1 ± 7.7*	*Yes (0.02)*
	0.15	-2.51 ± 1.52	194.8 ± 25	No (0.12)
Salinity	0.08	16 ± 4.8	-468 ± 165	Yes (0.001)
	0.23	*21.8 ± 3.8*	*-675 ± 130*	*Yes (8×10^{-8})*
	0.30	-42.41 ± 16.21	1609.3 ± 551	Yes (0.02)

Chlorophyll-*a*	0.025	-37 ± 26	84 ± 8.6	No (0.16)
	0.002	*-7 ± 20*	*62 ± 7*	*No (0.73)*
	0.01	77.83 ± 206	136 ± 31	No (0.71)

Table S1: Linear regression analysis results for each parameter against field observations of sea surface iodide for paramterisation Eq. (2) in standard font and Eq. (3) in italics, and grey shaded rows for Eq. (3a). R^2 represents the coefficient of determination (COD); the last column is a check for statistical significance at 5% with the p-value in parenthesis.