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Atmospheric Measurement Techniques
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Flow rate and source reservoir identification from airborne chemical sampling of the uncontrolled Elgin platform gas release

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Error analysis:

Method 1:

To calculate the error for method 1 we have

$$\ln C_z = \ln C_0 - \frac{z^2}{2\sigma_z^2} \qquad \text{(Eq S1)}$$

From the observations, the gradient is determined and then q found using the value of C_0 *and* σ_z obtained from the intercept and gradient, i.e. $q = f(\sigma_z, C_0)$. However, C_0 and σ_z are not truly independent, since in the majority of cases in (8) a change in C_0 is accompanied by a change in σ_z (if there is some constraint on the root-mean square error, RMSE, of the functional fit to the data). This functional relation of C_0 and σ_z suggests that traditional methods of error analysis are not appropriate in this case, and so we adopt a Monte-Carlo-simulation approach to determine the uncertainty in q. The method is as follows.

We denote the intercept of the line of best-fit in (8) as $\ln C_0 = \gamma$, with standard error E_γ and denote the gradient $(-1/2\sigma_z^2) = \mu$ with standard error E_μ. A large number (~5000) of unique straight-line fits were constructed, based upon γ, μ, E_γ and E_μ. We then calculate the mean $\overline{RMSE}$ (equivalent to the RMSE of the line of best fit) and standard deviation σ_{RMSE} of the RMSE for all of these fits and selected a large number (~1000) of these such that the RMSE of each individual fit is less than $\overline{RMSE} + \sigma_{RMSE}$ (this avoids combinations of intercept and gradient that lead to large RMSE values and would be considered poor fits to the data). From each line of best-fit, calculate σ_{z_k} and γ_k ($k = 1, \dots, k_{max}$; $k_{max} \sim 1000$).

The remaining parameters are sampled as follows. *(i)* We constructed a series of σ_{y_i} ($i = 1, \dots, i_{max}$; i_{max} ~1000)

$$\sigma_{y_i} = \overline{\sigma_y} + \sigma'_{y_i} \qquad \text{(Eq S2)}$$

The noise σ'_{y_i} is produced artificially from normally distributed random numbers and has zero mean, with a standard deviation corresponding to the standard error of the *observed* data; $\overline{\sigma_y}$ is the mean of the *observed* data. *(ii)* Similarly, we constructed a sample of wind speeds U_j ($j = 1, \dots, j_{max}$; j_{max} ~1000)

$$U_j = \overline{U} + U'_j \qquad \text{(Eq S3)}$$

Where, again, the noise U'_j is normally distributed noise with zero mean and standard deviation equal to the standard error of the *observed* data and $\overline{U}$ is the mean of the *observed* data (the observations here referring to the appropriate flight legs). The assumption is made here that the wind speed U_j and dispersion parameter σ_{y_i} are distributed normally; more sophisticated assumptions, such as that the wind speed obeys a Weibull-type distribution, would be possible but are not likely to affect significantly the results).

We then, computed the mean source of the $i_{max}\, j_{max}\, k_{max}$ (typically 10^9) reconstructed profiles:

$$\bar{q} = \frac{\sum_{i=1}^{i_{max}} \sum_{j=1}^{j_{max}} \sum_{k=1}^{k_{max}} \pi \sigma_{y_i} \sigma_{z_k} U_j e^{\gamma_k}}{i_{max}\, j_{max}\, k_{max}} \qquad \text{(Eq S4)}$$

The standard deviation of q is then calculated, based upon the $i_{max}\, j_{max}\, k_{max}$ individual samples of q and the mean $\bar{q}$, as calculated above.

Method 2:

To calculate the error for this method we have:

$$q = \sqrt{2\pi} C_0 U \sigma_y H \qquad \text{(Eq S5)}$$

Similar to the above, a series of sources is reconstructed. The wind speed *U* and dispersion parameter σ_y are sampled as for Method 1. In addition, a series of C_0 and *H* are produced:

$$C_{0_i} = \overline{C_0} + C'_{0_i} \quad (i=1, \ldots, i_{max}) \qquad \text{(Eq S6)}$$

$$H_l = \overline{H} + H'_l \quad (l=1, \ldots, l_{max}) \qquad \text{(Eq S7)}$$

where $\overline{C_0}$ and $\overline{H}$ are the mean of the observed concentrations and mixing-layer heights, respectively (in practice, there is only one value of *H* observed.) The added noise C'_{0_i} and H'_l is (as for Method 1) designed to have zero mean, and standard deviation equal to the observed variable. In the case of mixing-layer depth, this is taken to be 10% of the observed value, typically 100 m. Reconstructed sources are then taken to be

$$q_{i,j,k,l} = \sqrt{2\pi} C_{0_i} U_j \sigma_{y_k} H_l \qquad \text{(Eq S8)}$$

where the total number of samples $i_{max}\, j_{max}\, k_{max}\, l_{max}$ is taken to be of the order of a billion. The mean and standard deviation are then calculated in the usual manner.

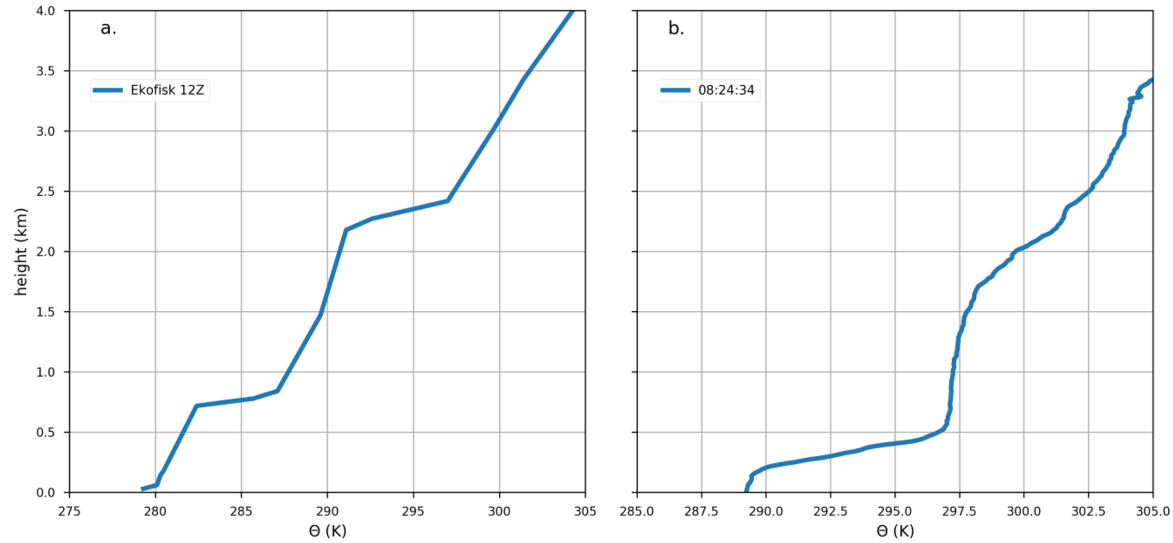

Figure S1: (a) radiosonde atmospheric profile taken from Ekofisk during the time of flight B688 (b) dropsonde atmospheric profile from flight B727.

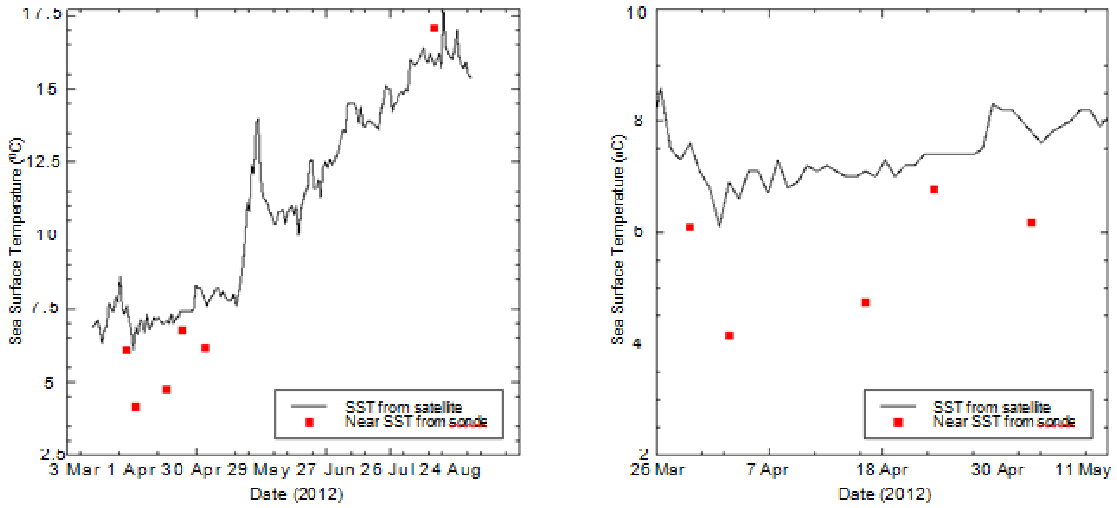

Figure S2: NOAA 100 km global Sea Surface Temperature (data-set derived from 8 km resolution satellite images) for the period of the flights. Air temperatures from radiosoundings and dropsondes.