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Interactive comment on "A mechanism for biologically-induced iodine emissions from sea-ice" *by* A. Saiz-Lopez and C. S. Boxe

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First, we would like to thank Rolf Sander for his most constructive comments on this manuscript; we answer the points in his second reply/report as follows:

1) On the first point regarding the use of Fick's law of diffusion in the model: We calculated an initial diffusion coefficient, based on an estimated flux (J), the initial concentration gradient, and the mean sea-ice thickness, using Fick's first law, yielding $D_{aq} \sim 8 \times 10^{-3}$ cm^2 s^{-1}. Upon utilizing Fick's second law we acknowledge misinterpreting the fact that the diffusion of the bulk medium (Daq) will not change although the flux (J) for the iodine species will vary with time. This misconception was due to the fact that we were calculating an estimated equation for the diffusion of D for iodine species.

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Nevertheless, following a decrease in the concentration gradient, as iodine accumulates in the QLL (Fig. 3b), the calculated Ddecreases very rapidly (i.e. first few hours time-scale) from our estimated initial value of 8 $\times$ 10^{-3} cm^2 s^{-1} to 1 $\times$ 10^{-5} cm^2 s^{-1}.

Therefore, following Rolf Sander's suggestion we have now conducted additional model simulations using a representative diffusion coefficient for water (i.e., Daq $\sim$ 10ˆ-5 cmˆ2 sˆ-1, as suggested by referee) and kept this diffusion coefficient constant, according to the formulation of Fick's laws. These additional model simulations were conducted with an initial flux (J), computed from Daq $\sim$ 10ˆ-5 cmˆ2 sˆ-1 and the initial iodine concentration gradient from the bottom to the top of the sea ice. Thereafter, we use Fick's second law to compute the change in concentration of iodine species, as iodine accumulates in the QLL (Fig. 3b), as a function of time (which we incorporate in Fick's first law to compute a flux (J) at each specified time (t) (see bellow for derivation)). Our model simulations show a small change in the timescale for iodine release to gas phase and a negligible change in the overall profiles for both gas and condense-phase species. This is due to the fact the release of gas-phase iodine species is governed by a combination of a flux from below (from micro- and macro-algal source) and, more importantly, the forward and reverse reaction rate constants that dictate the release of gas-phase I_2 from the brine layer. The results of the sensitivity runs will be included in the revised version of the paper.

In order to account for a changing concentration gradient with time and the corresponding iodine flux in the model we use the following Fick's law formalism:

Fick's first law is used in steady-state diffusion, i.e., when the concentration within the diffusion volume does not change with respect to time. In one (spatial) dimension, this is

$$J = -D\frac{\partial \phi}{\partial x} \tag{1}$$

where J is the iodine flux [molecules cm^2 s^{-1}], D is the diffusion coefficient [cm^2 s^{-1}], ϕ is the concentration [molecules m^{-3}], x is the sea-ice thickness [cm] and t is time

[s]. D is proportional to the velocity of the diffusing particles, which depends on the temperature, viscosity of the fluid and the size of the particles according to the Stokes-Einstein relation. The driving force for a one-dimensional diffusion is the concentration gradient term:

$$-\frac{\partial \phi}{\partial x} \tag{2}$$

Fick's second law is used in non-steady or continually changing state diffusion, i.e., when the concentration within the diffusion volume changes with respect to time.

$$\frac{\partial \phi}{\partial t} = D\frac{\partial^2 \phi}{\partial x^2} \tag{3}$$

It can be derived from the Fick's First law and the mass balance as follows:

$$\frac{\partial \phi}{\partial t} = -\frac{\partial}{\partial x}J = \frac{\partial}{\partial x}\left(D\frac{\partial}{\partial x}\phi\right) \tag{4}$$

Assuming the diffusion coefficient D to be a constant we can exchange the orders of the differentiating and multiplying by the constant:

$$\frac{\partial}{\partial x}\left(D\frac{\partial}{\partial x}\phi\right) = D\frac{\partial}{\partial x}\frac{\partial}{\partial x}\phi = D\frac{\partial^2 \phi}{\partial x^2} \tag{5}$$

and, thus, receive the form of the Fick's equations.

In order to solve Fick's Law, one initial condition and two boundary conditions are required. Two solutions to Fick's Law are generally used for numerical analysis of species in a fluid medium: infinite-source and limited-source diffusion. These are each described below. Here, as an approximation we incorporate the limited-source diffusion solution in our model. Given the following boundary conditions:

$\phi(x$,0) = 3 x 10ˆ-7 M

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$\int \phi(x,t)dx = S$

$\phi(x,\infty)$ = Iodine concentration in Phytoplankton colonies

Where S is called the “dose,” $S(t) = \phi_o(4Dt/\pi)^{1/2}$, where ϕ_o *is the initial concentration of iodine at the surface in the brine layer.*

The solution to Fick’s Law under these conditions is:

$$\phi(x,t) = (S/(\pi Dt)^{1/2}) \times \exp(-x^2/4Dt) \tag{6}$$

Therefore, at each time “*t*” “$\phi(x,t)$” was computed and then incorporated in Fick’s First law (Eq (1)) to calculate J at each specified time “t''. We used this approximation to take into account the change in J as a function of time as a result of a changing concentration gradient.

2) Regarding the terminology QLL *vs* brine layer: the QLL only pertains to pure water ice since the addition of solutes induce a freezing-point depression in water solutions below freezing point of pure water, thus forming a pure liquid (not a quasi-liquid) in equilibrium with ice. Therefore, lowering the temperature (or the freezing) of water solutions containing solutes (of variable concentration) below the melting point of pure water creates an interfacial or liquid-layer (in our case – a brine layer) that (at specified temperatures) is in equilibrium with the ice matrix portion. This interfacial liquid layer (brine layer) decreases with decreasing temperature as you approach the solutions eutectic point, where the entire matrix solidifies.

We will amend the terminology in the revised version of the paper. However, it is important to emphasize that to our knowledge, there has been no critical scientific analysis to accurately differentiate between a macroscopic and microscopic brine and quasi-liquid layer.