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Additional notes on the diffusion coefficient for a layered ice/humid air microstructure:

In what follows I provide some additional comments on the controversary over the role of hand-to-hand vapor transport as it relates to the diffusion coefficient in snow and/or layered ice/humid air microstructures.

Previously I provided a Technical Note on the subject of mass transfer in a layered ice/ humid air microstructure. The authors attempted to reject the Technical Note on the basis of a claimed improper derivation of the diffusion coefficient for this microstructure. Instead they argued that they had corrected the derivation and referenced Appendix C of Fourteau (2021). I then followed up with a discussion showing the validity of my derivation and, further, I pointed out the fundamental error they have made in their derivation.

The purpose of this Supplement is twofold. First, I want to add additional clarity, pointing out the very specific error in Appendix C of Fourteau (2021). Second, I am providing an appendix for addition to the Technical Note that lays to rest any further debate on the role of hand-to-hand mass transfer in the diffusion coefficient for the layered ice/humid air microstructure. It is interesting in that, after all the mind-bending exercises on complex equations, the entire discussion can be distilled down to just a few sketches with some supporting, relatively simple, equations.

I hope that I have struck the proper balance between being repetitive with prior remarks and leaving gaps in the development below. Apologies in advance if I have missed the mark.

The diffusion coefficient for the layered ice humid/air microstructure

In what follows, we restrict the discussion to ice volume fractions below 0.7 as it permits one to use simple expression with very high levels of accuracy, affording wonderfully easy comparisons between disparate views. Under this constraint, Hansen and Foslien (2015) show the diffusion coefficient for the layered microstructure is given by

$$D^{\mathrm{eff}} = \left(\frac{D_{\mathrm{v-a}}}{\phi_{\mathrm{ha}}}\right) \quad . \qquad (1)$$

It is worth noting that the above expression is precisely the diffusion occurring across the boundary of the unit cell, a point that is elaborated on in the Appendix below.

The authors have argued that the above equation is “invalid” and claim to have corrected the derivation in Appendix C (Fourteau, 2021), leading to an equation given by

$$D^{\mathrm{eff}} = D_{\mathrm{v-a}} \quad . \qquad (2)$$

In their effort to support this view, they argue that the volume averaged diffusion (by their reasoning) supports this expression—much more on this point is found in the Appendix below.

In my previous note discussing this article, I have provided the precise point in Appendix C of Fourteau (2021) where the authors have gone awry in their development. In brief, the authors write: "The heat flux q^{cond} through the sole process of conduction is thus given by" (using my notation)

$$q^{\text{cond}} = \phi_{\text{i}} k_{\text{i}} \left(\frac{\partial\theta}{\partial\xi}\right)_{\text{i}} + \phi_{\text{ha}} k_{\text{ha}} \left(\frac{\partial\theta}{\partial\xi}\right)_{\text{ha}} \tag{3}$$

The diffusion coefficient is then developed by recognizing the latent heat flux contribution is given by $q - q^{\text{cond}}$.

On the surface, Eq. (3) has the appearance of a valid approach, yet, it is not valid in the case of diffusion. The authors introduce Eq. (3) in an effort to isolate conduction from diffusion as energy transfer mechanisms. However, the error arises in that the constituent temperature gradients they substitute into Eq. (3) are based on the fully coupled solution involving heat conduction and diffusion, i.e., diffusion is inherently built into analysis and, further, it very much affects the constituent temperature gradients. As a result, and the authors have not isolated q^{cond} as they have claimed. The proper way to account for q^{cond} is to set the diffusion to zero and compute the thermal conductivity as, for example, done in Calonne (2011) and Riche and Schneebeli (2013). As a result of the improper calculation of q^{cond}, the problem immediately cascades to an incorrect calculation of the latent heat and, further, the diffusion coefficient.

By improperly deriving the diffusion coefficient for this microstructure, the defining argument the authors provide against the Technical Note can be dismissed.

Appendix B

A final word on the mathematical and physical role of hand-to-hand vapor transport in the diffusion coefficient for snow

Mass transfer in a layered ice/humid air microstructure under the influence of a macroscale temperature gradient can be elegantly captured with a few simple sketches and supporting equations. Begin with Figure 1, showing a layered ice/humid air microstructure under a temperature gradient and an accompanying unit cell for the structure. Vapor diffusion vectors across the exposed upper surface of the unit cell are also shown.

The mass flux moving through the humid air of the unit cell is given by the expression

$$j = \gamma_{\text{v}} \, v_{\text{v}} = -\frac{D_{\text{v-a}}}{\phi_{\text{ha}}} \left(\frac{d\,\gamma_{\text{v}}}{d\,\theta}\right) \frac{\partial\theta}{\partial x} \quad . \tag{B.1}$$

where $\frac{\partial\theta}{\partial x}$ is the macroscale temperature gradient.

This mass flux is also the surface flux leaving the top of the unit cell and the surface flux arriving at the bottom of the unit cell through deposition of water vapor and the resulting accumulation of ice. The surface flux is not in dispute and was first derived by de Quervain (1963).

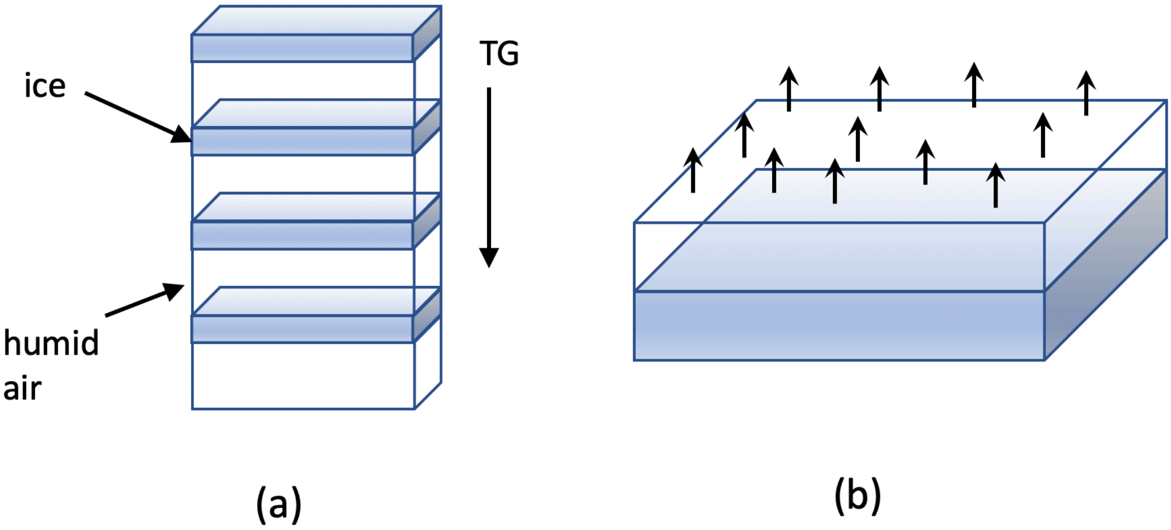

Figure 1. (a) Layered ice/humid air microstructure subjected to a temperature gradient. (b) Unit cell showing mass flux across the upper surface. The same mass flux is depositing on the lower surface through condensation.

The surface flux across the top or bottom of the unit cell is precisely the mass flux for the macroscale structure of Figure 1a, as water vapor moves continuously from the top of one unit cell to the bottom of the next and so on.

On the other hand, the authors wish to define mass flux through the system as the volume average of Eq. (B.1) for the unit cell, leading to a flux of

$$j = \gamma_{\mathrm{v}}\, v_{\mathrm{v}} = -\, D_{\mathrm{v-a}} \left(\frac{d\,\gamma_{\mathrm{v}}}{d\,\theta}\right)\frac{\partial\theta}{\partial x} \tag{B.2}$$

Now one must rely on the true definition of mass flux. Without question, mass flux is the amount of mass per unit area per unit of time *moving across a surface*. So, without delving into any mathematics, the physics of the controversary is clearly exposed. The surface flux of Eq. (B.1) is, indeed, the true mass flux leaving one unit cell and entering the next adjacent unit cell. This is occurring throughout every unit cell.

So why does the volume averaging technique of Eq. (B.2) produce a different result from the surface flux of Eq. (B.1)? Certainly, proper volume averaging of the mass flux must agree with the surface flux. The definitive answer is the glaring omission of the effects of hand-to-hand vapor transport. In the Technical Note, I used the concept of an infinite ice velocity, the source/sink phenomenon, to show the apparent velocity of water vapor through the entire unit cell was given by

$$v_{\mathrm{v}}^{*} = \frac{v_{\mathrm{v}}}{\phi_{\mathrm{ha}}} \quad . \qquad \text{(B.3)}$$

For those who find the above argument a bit too abstract or non-physical for their liking, Hansen (2019) reached the same result by simply showing that water vapor, using the standard definition of vapor velocity, is effectively moving through the system at the apparent velocity given by Eq. (B.3) because of the shortened diffusion path through the humid air. One can readily see this by examining Figure 2 showing a very high ice volume fraction. The simple question to pose is: "how long does it take a water molecule to reach the upper surface as compared to traversing through a unit cell of humid air only?" The answer is explained by Eq. (B.3). Once one recognizes the apparent velocity (perhaps effective velocity is a better term), the volume average of the mass flux leads identically to the surface flux of Eq. (B.1).

In discussing hand-to hand vapor transport the authors have often used the term nonphysical to describe this mass transport mechanism, e.g., "The reliance on the hand-to-hand mechanism that instantly transports water molecules through the ice phase, which is not a real physical phenomenon." On the contrary, what is truly nonphysical, and non-mathematical, is to have the volume average mass flux and the surface mass flux across a unit cell boundary in disagreement.

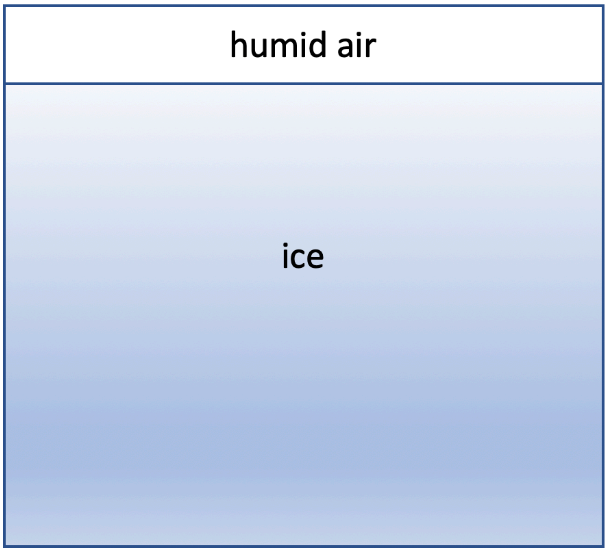

Figure 2. High volume fraction ice constituent for a unit cell. The shortened distance water vapor must travel compared to a unit cell of humid air only is immediately apparent.

By incorporating hand-to-hand vapor transport, the stars align and we have perfect agreement for the following:

- Surface flux across a unit cell boundary
- Volume averaged mass flux
- Macroscale mass flux developed from first principles

Of course, all of this information runs counter to the authors' narrative that the diffusion coefficient in the layered ice/humid air microstructure and, by extension, the diffusion coefficient in snow is less than one (Fourteau, 2021). The physics and mathematics simply do not support their view.

When hand-to-hand diffusion is properly accounted for, numerical evidence points toward a slight enhancement in the effective diffusion coefficient for snow. These include the works of Christon (1994), remarkable for the time period, and Pinzer (2012). As I pointed out in my original comment of this article, the authors' present calculations of the diffusion coefficient will likely show the same slight enhancement in the normalized diffusion coefficient when hand-to-hand diffusion is properly accounted for. Moreover, these numerical calculations are remarkably consistent with the diffusion model of Foslien (1994).