Figure 1: Diffusive mixing between two boxes.

1 What is mixing, and what is diffusion?

Let's assume we have two identical boxes of length Δz with cross section A touching each other, see Fig. 1. The total number of a certain kind of molecules in one of those boxes is

$$N = n \, A \, \Delta z \tag{1}$$

where n [cm^{-3}] is the molecular particle density. From the 3D hydro model, we observe that matter goes up and down with some average (e.g. root-mean-square) velocity [cm/s] as

$$v = v_{z,\text{rms}} = \sqrt{\langle v_z^2 \rangle_t} = \sqrt{\langle v_z^2 \rangle_{\text{vol}}} \tag{2}$$

which either requires some kind of long-term average over time t or a spatial average over some suitably large volume. But there is no bulk motion, otherwise it's an advection problem! We are talking here about a mixing/diffusion problem, i.e. $\langle v_z \rangle_t = \langle v_z \rangle_{\text{vol}} = 0$.

Because of the random mixing motions, molecules will go from box 1 to box 2 and vice versa. The associated mean particle fluxes [cm^{-2}s^{-1}] through the contact area A are

$$j_1 = n_1 \, v \qquad \text{rightwards} \tag{3}$$
$$j_2 = n_2 \, v \qquad \text{leftwards.} \tag{4}$$

The change of the total number of molecules N_1 in the left box is

$$dN_1 = -j_1 \, A \, dt + j_2 \, A \, dt = (n_2 - n_1) \, v \, A \, dt \tag{5}$$
$$\Rightarrow \frac{dn_1}{dt} = \frac{n_2 - n_1}{\Delta z} v \;\rightarrow\; -\frac{\partial n}{\partial z} v \tag{6}$$

Diffusion with rate equations: The problem can be re-formulated with rate constants $R = v/\Delta z$ [1/s], like a chemist would do

$$\frac{dn_1}{dt} = -n_1 R + n_2 R \tag{7}$$
$$\frac{dn_2}{dt} = -n_2 R + n_1 R \tag{8}$$

The mixing timescale: Let's assume box 1 is full, and box 2 initially has none of those molecules. How long would it take to empty box 1? From Eq. (7), with $n_2 \to 0$, we find $n_1(t) = n_1(0) \exp(-t/\tau_{\text{mix}})$ where

$$\boxed{\tau_{\text{mix}} = \frac{1}{R} = \frac{\Delta z}{v}} \tag{9}$$

The same result is obtained when considering the right box (index 2). In `static_weather`, we replenish all distant boxes as

$$\frac{dn_2}{dt} = \frac{n_1 - n_2}{\tau_{\text{mix}}} \tag{10}$$

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where index 1 refers to the "full" box which ultimately provides the supply of fresh condensible material at some distance. Solving that mixing ansatz (Eq. 10) for the mixing timescale results in

$$\tau_{\text{mix}} = \frac{n_1 - n_2}{\frac{dn_2}{dt}} = \frac{n_1 - n_2}{-n_2 R + n_1 R} = \frac{1}{R} \tag{11}$$

without having to assume anything for n_1 or n_2.
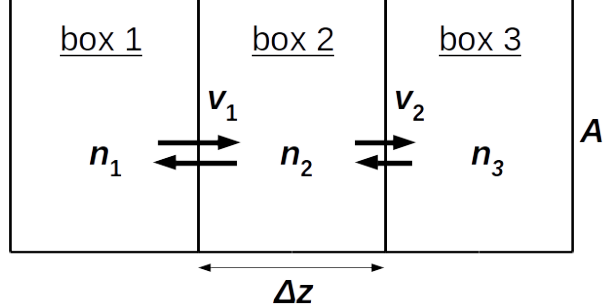
2   A linear chain of boxes

Figure 2: Diffusive mixing between three boxes.

Let us now repeat the same thought experiment for 3 boxes in a row as sketched in Fig. 2. The rate equations in this case, with $R_1 = v_1/\Delta z$ and $R_2 = v_2/\Delta z$ are

$$\frac{dn_1}{dt} = -n_1 R_1 + n_2 R_1 \tag{12}$$

$$\frac{dn_2}{dt} = n_1 R_1 - n_2 (R_1 + R_2) + n_3 R_2 \tag{13}$$

$$\frac{dn_3}{dt} = -n_3 R_2 + n_2 R_2 \tag{14}$$

Closer inspection of Eq. (13) shows the analogy to Fick's laws

$$\frac{dn_2}{dt} = \frac{n_1 - n_2}{\Delta z} v_1 + \frac{n_3 - n_2}{\Delta z} v_2 \tag{15}$$

$$\rightarrow \quad \frac{\partial}{\partial z}\left(\frac{\partial n}{\partial z} v\right) \Delta z = \frac{\partial}{\partial z}\left(D \frac{\partial n}{\partial z}\right) , \tag{16}$$

where we find the diffusion constant [cm^2/s] (velocity $\times$ length) to be

$$\boxed{D = v \, \Delta z} \tag{17}$$

The meaning of Δz is a bit special in Eq. (17). The mixing motions typically have a certain intrinsic range ℓ, before the incoming particles actually have an effect on the concentration in the box. When $\Delta z \ll \ell$, those particles simply rush through, there is no time to mix with the ambient gas in the box. In the opposite case, when $\Delta z \gg \ell$, those particles only enrich the regions close to the surface A, but not in the entire box, the concentration gradient on the box is substantial, and that local enhancement at the surface should actually be taken into account when we determine the flux backwards to the originating cell, which we do not. Therefore, the only box thickness where the local Eq. (17) actually works fine is when

$$\text{Diffusion:} \quad \Delta z \approx \ell . \tag{18}$$

Indeed, when determining diffusion constants, we must always make some kind of assumption about ℓ, for example $\ell \sim$ the mean free path for gas-kinetic diffusion, or $\ell \sim H_p$ for convective mixing, where H_p is the scale height.

However, for our "global mixing approach", we actually do not need such an assumption. To find the mixing timescale τ_{mix} for the 3-box experiment, we assume that the concentration n_2 in the sandwich box 2 adjusts quickly to n_1 and n_3. Setting the time derivative in Eq. (13) to zero we find

$$n_2 = \frac{n_1 R_1 + n_3 R_2}{R_1 + R_2} \tag{19}$$

Generalising the derivation of τ_{mix} from the 2-box experiment,

$$\tau_{\mathrm{mix}}^{-1} = -\frac{1}{n_1}\frac{dn_1}{dt} = -\frac{1}{n_1}\Big(-n_1 R_1 + n_2 R_1\Big) \tag{20}$$

and using Eq. (19) we find

$$\tau_{\mathrm{mix}} = \frac{R_1 + R_2}{R_1 R_2}\,\frac{1}{1 - n_3/n_1}\ , \tag{21}$$

which, in the limiting case of $n_3 \to 0$, results in

$$\boxed{\tau_{\mathrm{mix}} \;\to\; \frac{1}{R_1} + \frac{1}{R_2} \;=\; \frac{\Delta z}{v_1} + \frac{\Delta z}{v_2}}\ . \tag{22}$$

Again, the same result is obtained when considering the right box (index 3) and using Eq. (19)

$$\tau_{\mathrm{mix}} = \frac{n_1 - n_3}{\frac{dn_3}{dt}} = \frac{n_1 - n_3}{-n_3 R_2 + n_2 R_2} = \frac{\Delta z}{v_1} + \frac{\Delta z}{v_2}\ . \tag{23}$$

This thought experiment can be extended to a linear chain of boxes of arbitrary length K. For each chain length, we consider n_1 and n_K to be given and assume that $n_2 \ldots n_{K-1}$ can be calculated in their stationary limits. This is similar to the *Maxwell daemon* in nucleation theory, who would always collect the large clusters, break them up into monomers, and return them this way back to the gas phase. Here, we need a daemon who makes sure that n_K stays small, and n_1 stays large. That deamon would quickly transport the molecules arriving in the right box back to the left box, to create a stationary problem with constant diffusive fluxes through all interface areas. In our case, the deamon is dust formation and settling, causing a stationary situation.

Assuming $n_K \to 0$, the result is[1]

$$\boxed{\tau_{\mathrm{mix}} \;=\; \frac{1}{R_1} + \frac{1}{R_2} + \ldots + \frac{1}{R_{K-1}} \;=\; \frac{\Delta z}{v_1} + \frac{\Delta z}{v_2} + \ldots + \frac{\Delta z}{v_{K-1}}} \tag{24}$$

The same result is obtained for the mixing timescale of the right box

$$\tau_{\mathrm{mix}} = \frac{n_1 - n_K}{\frac{dn_K}{dt}} = \ldots = \frac{\Delta z}{v_1} + \frac{\Delta z}{v_2} + \ldots + \frac{\Delta z}{v_{K-1}}\ . \tag{25}$$

In the limiting case $\Delta z \to 0$, the final result is

$$\boxed{\tau_{\mathrm{mix}}(z) \;=\; \int_0^z \frac{1}{v(z')}\,dz'} \tag{26}$$

which shows that the result is independent of the choice of Δz (disregarding here the uncertainties in the actual numerical computation of that integral).

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[1] I checked 4 boxes and 5 boxes with Mathematica

This result makes a lot of sense to me:

- Equation (26) states an expression for τ_{mix} that *matches its definition and use.* It is the replenishment timescale in consideration of a distant supply.

- The mixing timescale is monotonic increasing with z, i.e. it always takes longer to replenish an atmospheric layer which is higher above the ground.

- There can be a bottleneck. If there is a region between 0 and z where $v(z')$ is very slow, all regions above that region should indeed receive very little mixing supply. This is likely to cause some numerical problems when trying to evaluate the integral, as locally, there might be a point where v is very close to zero.

- If $v = \text{const}$, Eq. (24) agrees with the 2-box result (Eq. 9) and the 3-box result (Eq. 22), namely $\tau_{\text{mix}}(z) = z/v$.

3 A relation between $D(p)$ and $\tau_{\text{mix}}(p)$?

Ludwig et al. (2002) have derived an expression for the "mass exchange timescale" from time-dependent 3D numerical models for late M-dwarf atmosphere, using passive tracer particles, as

$$\ln \tau_{\text{mix}}(p) = \ln \tau_{\text{mix}}(p_0) + \beta \ln \left(\frac{p_0}{p} \right) \tag{27}$$

with $\beta \approx 2.2$. The question is the following is: Can we find an expression for the diffusion coefficient $D(p)$ that would agree with Eq. (27)? One approach to prescribe the diffusion coefficient in astrochemical models is

$$D(p) = D_0 \left(\frac{p}{p_0} \right)^{\alpha} \tag{28}$$

where $\alpha = 0$ (constant diffusion coefficient) and $\alpha = -0.5$ (diffusion coefficient increases with height) are popular choices. What would such a diffusion coefficient mean for the mass exchange timescale?

A problem with our Eq. (26) is that $\tau_{\text{mix}} \to 0$ at $z = 0$. If the reservoir is assumed to be located at $z = 0$, well then it would exchange itself extremely rapidly, but what we are looking for is rather how the mass exchange timescale increases from a given value

$$\tau_{\text{mix}}(p) = \tau_{\text{mix}}(p_0) + \int_{\ln p_0}^{\ln p} \frac{1}{v(p)} \left(-H \, d\ln p \right) \tag{29}$$

where I have used hydrostatic equilibrium $d\ln p = -dz/H$ to substitute from z to $\ln p$, H is the scale height assumed to be constant here. Equation (29) considers the reservoir to exchange with is situated deeper than $z = 0$, and assumes that we know it at p_0. With the ansatz Eq. (26) and $D(p) = H \, v(p)$ we get

$$
\begin{aligned}
\tau_{\text{mix}}(p) &= \tau_{\text{mix}}(p_0) - \frac{H^2}{D_0} \int_{\ln p_0}^{\ln p} \left(\frac{p}{p_0} \right)^{-\alpha} d\ln p & (30) \\[2mm]
&= \tau_{\text{mix}}(p_0) - \frac{H^2}{D_0} \int_{\ln p_0}^{\ln p} \exp \left(-\alpha \ln \left(\frac{p}{p_0} \right) \right) d\ln p & (31) \\[2mm]
&= \tau_{\text{mix}}(p_0) + \frac{H^2}{\alpha \, D_0} \left(\left(\frac{p}{p_0} \right)^{-\alpha} - 1 \right) & (32) \\[2mm]
&= \tau_{\text{mix}}(p_0) + \frac{H^2}{\alpha} \left(\frac{1}{D(p)} - \frac{1}{D_0} \right). & (33)
\end{aligned}
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There is no simple way to use Eq. (27) to determine α from β. However, there are some interesting limiting cases for $p \ll p_0$. When $\alpha < 0$, i.e. $D(p) \gg D_0$, then $\tau_{\mathrm{mix}}(p)$ eventually becomes constant

$$\alpha < 0 \quad \Rightarrow \quad \tau_{\mathrm{mix}}(p) \ \to \ \tau_{\mathrm{mix}}(p_0) \ + \ \frac{H^2}{\alpha\, D_0} \tag{34}$$

which makes sense. As the diffusion gets faster and faster, τ_{mix} is given by the time the matter needs to diffuse through the low bottleneck. For $\alpha = 0$, we use Eq. (31) to find the solution

$$\alpha = 0 \quad \Rightarrow \quad \tau_{\mathrm{mix}}(p) \ = \ \tau_{\mathrm{mix}}(p_0) \ + \ \frac{H^2}{D_0} \ln\left(\frac{p_0}{p}\right) \tag{35}$$

Both cases do not have a shape that would allow us to determine α from β in Eq. (27), not even in the limiting case $p \ll p_0$. However, when $\alpha > 0$ then $\tau_{\mathrm{mix}}(p_0)$ becomes unimportant for $p \ll p_0$ and we find

$$\alpha > 0 \quad \Rightarrow \quad \tau_{\mathrm{mix}}(p) \ \to \ \frac{H^2}{\alpha\, D_0} \left(\frac{p_0}{p}\right)^{\alpha} \tag{36}$$

from which we can conclude

$$\alpha > 0 \quad \Rightarrow \quad \ln \tau_{\mathrm{mix}}(p) \ \to \ \mathrm{const} \ + \ \alpha \ln\left(\frac{p_0}{p}\right) . \tag{37}$$

Compared to Eq. (27) for $p \ll p_0$ we find $\alpha = \beta$.

But anyway, if we want to assume a powerlaw for the diffusion const (Eq. 28), it would be consequent to compute the mass exchange timescale in `StaticWeather` as

$$\boxed{\tau_{\mathrm{mix}}(p) \ = \ \tau_{\mathrm{mix}}(p_0) \ + \ \frac{H^2}{\alpha} \left(\frac{1}{D(p)} - \frac{1}{D_0}\right)} \tag{38}$$

(when $\alpha = 0$, then Eq. (35) should be used instead).

References

LUDWIG, H.-G., ALLARD, F., HAUSCHILDT, P. H. (2002, November). Numerical simulations of surface convection in a late M-dwarf. *A&A* **395**, 99–115.