Pheromone output of a simple olfactometer

Thomas Nowotny
Centre for Computational Neuroscience and Robotics
University of Sussex
Falmer, Brighton BN21 9QJ
UK

Jean-Pierre Rospars

Co-author 3

10-04-2008

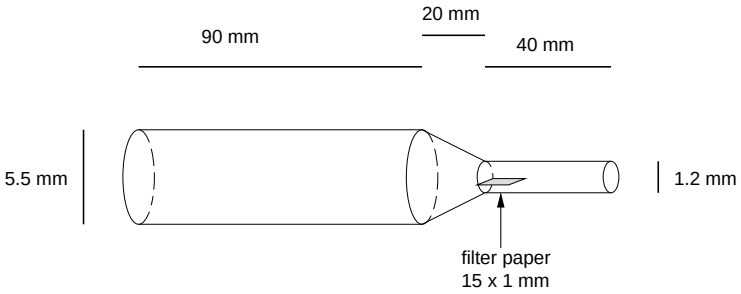

Figure 1: Geometry of the cartouche de stimulation: We assume for simplification that it is cylindrical for most of its length and contracts in a straight line in between. The inside diameters are exact at the ends.

1 Introduction

In this second version of calculating the output of an olfactometer I use Jean-Pierres description of the stimulation apparatus but still completely arbitrary values for de- and adsorption rates and the diffusion constant. This time the treatment is based on numerical simulations taking an approximate geometry into account (Fig. 1). A realistic geometry could easily be substituted. The results mainly confirm earlier experiments showing mainly linear dependencies of the total amount of pheromone delivered on both number of deposited molecules and air speed, with some (small) deviations in the latter dpeendence.

2 Method

The basic geometry for the "cartouche de stimulation" is shown in figure 1. We discretize the cartouche de stimulation into thin compartments which are assumed to have homogenous pheromone density. The pheromone is deposited on a 15×1 mm filter paper and starts to desorb into the air in the cartouche. It then can diffuse between compartments and be moved by the air stream when it is switched on during stimulation. Accordingly, the equations for a compartment not at one of the ends of the cartouche are (also see figure 2)

$$\frac{dN_{\beta i}}{dt} = -\Big(\frac{A_{i-1}}{A_i \Delta x}\kappa + \frac{\kappa}{\Delta x} + \frac{v_V}{A_i \Delta x}\Big) N_{\beta i} \tag{1}$$

$$+ \Big(\frac{\kappa}{\Delta x} + \frac{v_V}{A_{i-1}\Delta x}\Big) N_{\beta i-1} \tag{2}$$

$$+ \frac{A_i}{A_{i+1}\Delta x}\kappa N_{\beta i+1} \tag{3}$$

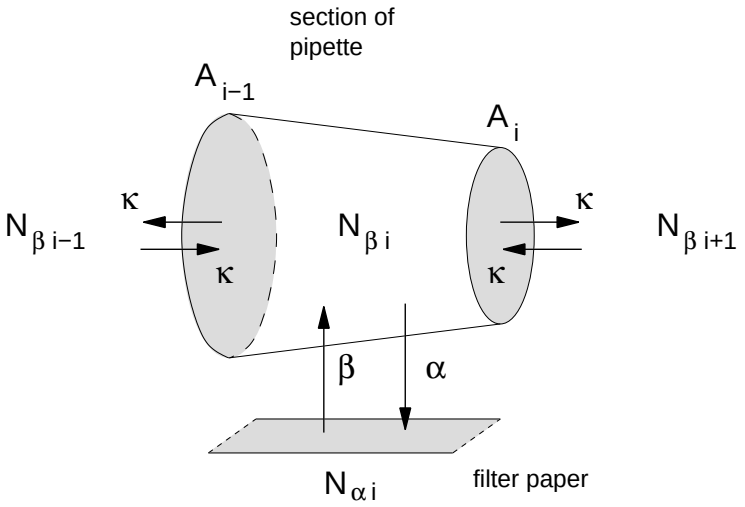

Figure 2: Illustration of the simulation.

if not containing filter paper and with additional terms

$$\frac{dN_{\beta i}}{dt} = \ldots - \alpha N_{\beta i} + \beta N_{\alpha i} \tag{4}$$

$$\tag{5}$$

if the filter paper is in the compartment ($i = 110 \ldots 124$). For the molecule number on the filter paper we have the corresponding equation

$$\frac{dN_{\alpha i}}{dt} = \alpha N_{\beta i} - \beta N_{\alpha i}. \tag{6}$$

$$\tag{7}$$

For the endpieces we choose the following boundary conditions: At the left no pheromone can diffuse in or out, but fresh air enters during stimulation:

$$\frac{dN_{\beta 0}}{dt} = -\Big(\frac{\kappa}{\Delta x} + \frac{v_V}{A_0 \Delta x}\Big) N_{\beta 0} \tag{8}$$

$$+ \frac{A_0}{A_1 \Delta x} \kappa N_{\beta 1}. \tag{9}$$

On the right end, the pheromone can leak out but is not diffusing back in (approximately infinite volume of the space outside the cartouche):

$$\frac{dN_{\beta N-1}}{dt} = -\Big(\frac{A_{N-2}}{A_{N-1}\Delta x}\kappa + \frac{\kappa}{\Delta x} + \frac{v_V}{A_{N-1}\Delta x}\Big) N_{\beta N-1} \tag{10}$$

$$+ \Big(\frac{\kappa}{\Delta x} + \frac{v_V}{A_{N-2}\Delta x}\Big) N_{\beta N-2}. \tag{11}$$

In these equations A_i are the crossection areas of the cartouche, each compartment delimited by A_{i-1} on the left and A_i on the right. They are chosen according to the geometry shown in figure 1. The 150 compartments of 1 mm width are integrated with an explicit 5/6 order Runge Kutta algorithm.

The initial conditions are that the pheromone is all adsorbed to the filter paper, $N_{\alpha i}(0) = N_0/15$, $i = 110, \ldots, 124$ and no pheromone is in the air, $N_{\beta i}(0) = 0$, $i = 0, \ldots, 149$.

3 Results

We simulated a protocol in which the filter paper loaded with pheromone is inserted into the cartouche at time 0 and then pheromone diffuses in the cartouche for 60 s. Then, for 200 ms an air stream of 10 l per second is turned on that "puffs" the pheromone/air blend out of the right end of the cartouche. Afterwards diffusion without drift resumes.

3.1 General shape of distributions

First we explored the distribution of pheromone in the cartouche over time due to de- and adsorption, diffusion and eventually the air puff during the stimulation. We used a deposit of $2.23 \cdot 10^9$ molecules and an air speed of 10 l/hour $\approx 2.778 \cdot 10^{-6}$ m^3/s. For diffusion rate and de- and adsorption rate we used the (as of now arbitrarily guessed) values: $\kappa = 10^{-2}$ m/s, $\beta = 0.1$ 1/s, and $\alpha = 10^{-3}$ 1/s. The results are illustrated in figures 3 and 4 for 5 s time steps and 0.01 s time steps around $t = 60$ s. The distribution is bell shaped as expected and then moved out of the cartouche quickly when the air stream is turned on. The somewhat odd shape on the left flank of the distribution is due to shape of the cartouche.

As a measure of pheromone delivery we can calculate the rate of molecules pre second that leave the cartouche at any given time. The result is illustrated in figure 5. Panel A shows the exit rate for the whole experiment on a log scale, which shows a clear leakage of pheromone prior to the proper puff which is, however, about 4 orders of magnitude lower than the exit rate during the puff.

Panel B sohws the rate of pheromone exiting during the puff. It is noticeable that the exit rate increases strongly at the beginning but stabilizes at about half maximum value during the second half of the puff.

3.2 Dependence of pheromone delivery on deposit size and air speed

Having the simulation well-established we proceeded to measure the dependence of delivered pheromone on the number of deposited pheromone molecules and on the ai speed during the puff. Figure 6 illustrates the results. Pheromone delivery can be measured as peak delivery rate or as total number of molecules delivered. We show data for both.

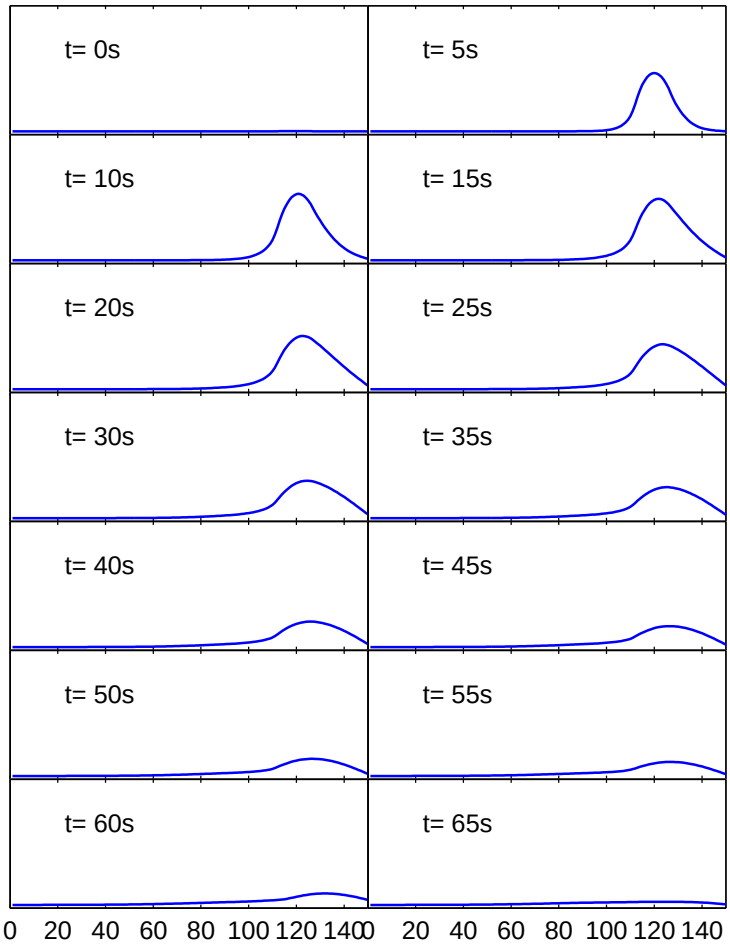

Figure 3: Profiles of pheromone concentration (molecules/m^2) in the cartouche de stimulation over time assuming fairly fast desorption and diffusion. The left end is closed (see equation (9)). The right end is open so that pheromone can leak out but no pheromone comes back in (assumption of an infinite volume outside). The kinks in the shape of the profile are caused by the diameter changes in the pipette according to figure 1.

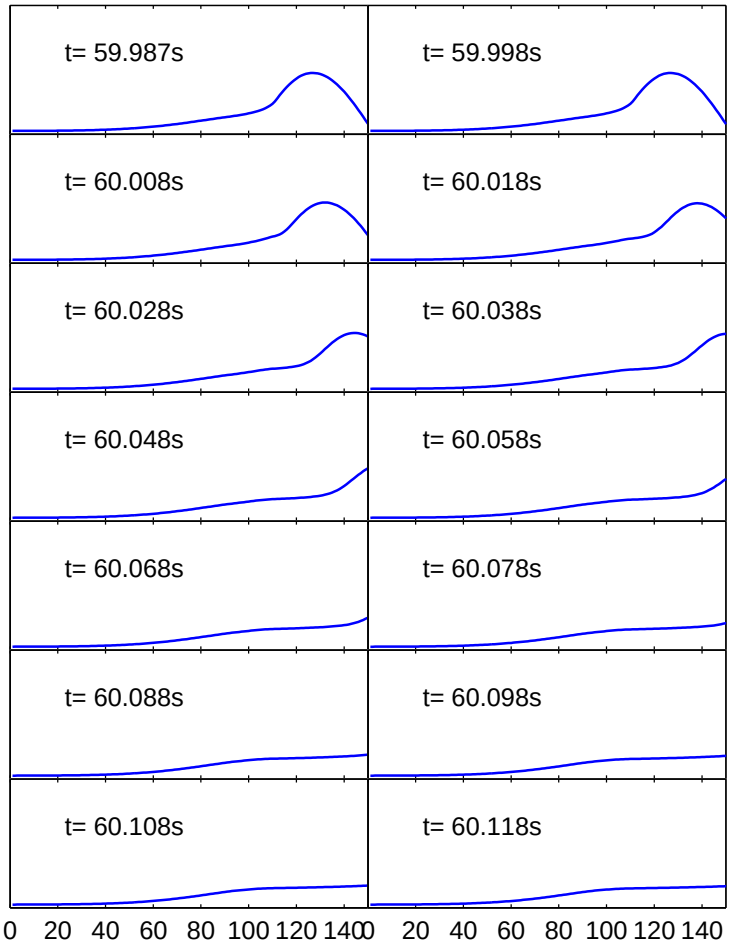

Figure 4: Profiles at the times around the puff. One sees how the concentration profile if just pushed through the pipette to the right. After the puff the pheromone continues to leak out (not shown here).

As a function of the deposited number of molecules the maximum exit rate is perfectly linear (Pearsons correlation $\rho \approx 1$ with pvalues $< 10^{-40}$), see figure 6A. Data was taken over many orders of magnitude.

A similar picture presents itself for the total number of molecules in the puff (Fig. figuredependence2A). Here, again the pvalues are almost 0 indicating perfectly linear dependence.

When we fix the number of deposited molecules and vary the airspeed of the puff (Fig. 6B and 7B) we see that the maximal rate of ejected pheromone is very linearly increasing with increasing airspeed. The figure shows the maximum rate of exiting molecules in molecules/s.

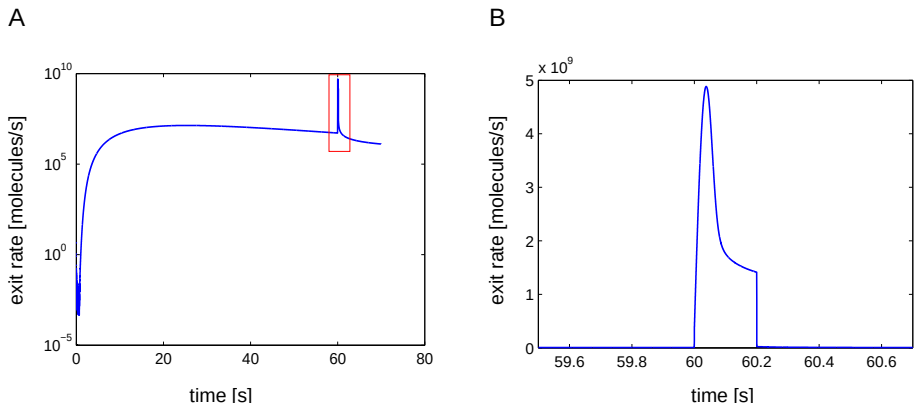

Figure 5: Rate of pheromone exiting the cartouche de stimulation (molecules/s). A) logarithmic plot demonstrating the leakage before and after the puff. B) temporal high resolution picture of the puff itself. Clearly the puf is by no means a square profile.

For the total number of ejected molecules we observe with growing airspeed a somewhat damped increase for higher speeds. Here, the data is normalized by the total number deposited molecules which collapses the curves exactly onto one.

Note that this measures only the molecules ejected in the time interval $[60, 60.2]$ s and may not reflect the total number of molecules escaping in the whole experiment (additional molecules exit by diffusion when the airstream is off).

As one interesting detail we note that the time of the maximal exit rate changes with the airspeed but not with the number of deposited molecules (Fig. 8).

4 Summary by Jean-Pierre

4.1 MAIN RESULTS

In summary your realistic model of our stimulating apparatus shows that:

1. The temporal profile of the pheromone puff presents a distinct peak with quick rise and decline followed by a shoulder with slower decline (Fig. 4B).

2. The maximal exit rate (height H of the peak in molecule/s) is proportional to the number N_0 of molecules deposited on the filter paper (Fig. 5A) and to the air speed v (Fig. 5B).

3. The number N of molecules blown out during the puff is proportional to N_0 (Fig. 6A) and to the air speed (Fig. 6B), except a different slope at very low airspeed.

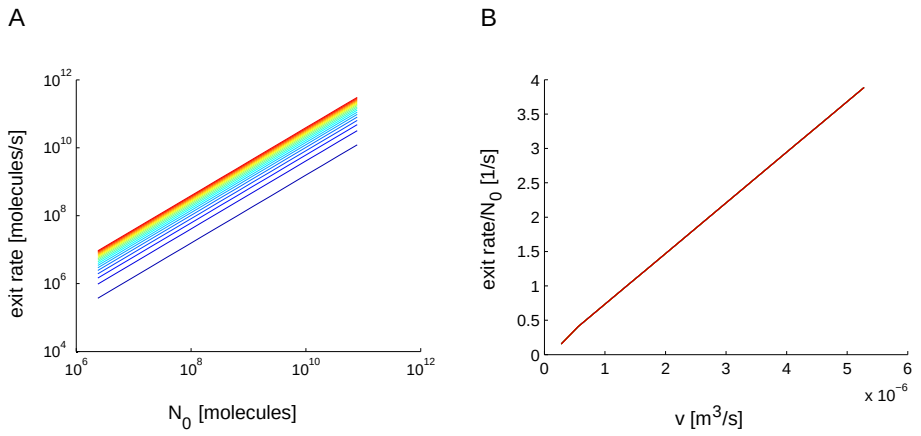

Figure 6: Dependence of the maximal exit rate from the cartouche (which occurs during the puff) in dependence on the number of molecules deposited (A) and for fixed numbers of deposited molecules in dependence on the air speed of the puff (B). In (B) we normalized by the number of deposited molecules, N_0, which collapses all curves onto a single line.

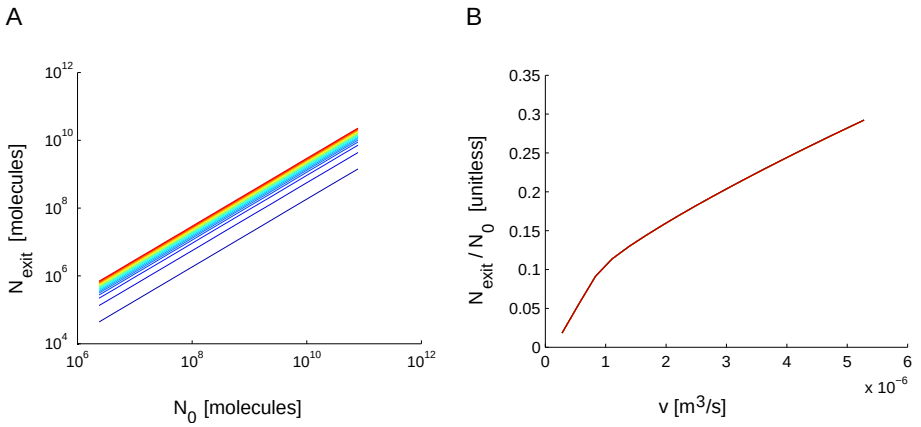

Figure 7: Dependence of the number of pheromone molecules exiting the cartouche during the puff (between 60 s and 60.2 s) in dependence on the number of molecules deposited (A) and for fixed numbers of deposited molecules in dependence on the air speed of the puff (B). In (B) we normalized by the total number of deposited molecules, which collapses all curves onto a single line because of the exact linear dependence on N_0. It is interesting to see how small the percentage of actually released pheromone is (order of magnitude of 30 %).

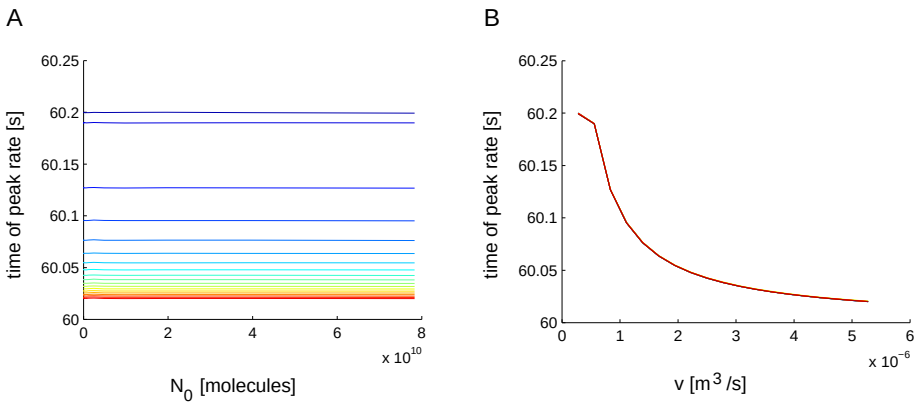

Figure 8: Time of occurence of the maximal rate of molecules exiting the cartouche de stimulation. A) in dpendence on the number of dpeosited molecules at a set of fixed airspeeds and B) as a function of the airspeed at fixed amounts of deposited pheromone. Because the peak time does not depend on the amount of pheromone deposited, all curves are identical.

Conclusion: You essentially confirm the expected relation $N_{\text{exit}} = kN_0v$ and you add another one $H = KN_0v$, where H is the pheromone flux (molecule/s) at the peak. This is a very nice conclusion.

4.2 OTHER RESULTS

You provide other interesting results:

4. You confirm the existence of a permanent leak and you give an estimation of its importance with respect to the peak (Fig. 4A). A pollution results from this leak which may deserve some attention.

5. You give the full profile of pheromone concentration along the Pasteur pipette (from 0 to 15 cm) at different times (from 0 to 65 s) in still air (Fig. 2), and how the pheromone cloud is pushed out of the pipette by the air puff (Fig. 3).

6. You show that the time of occurrence of the peak depends on v but not on N_0 (Fig. 7A).

4.3 SUGGESTIONS

I have a few suggestions: (italics are Thomas answers)

1. Your document is so interesting that I'd like you make it more readable by adding the axes labels (and units) and the letters A and B inside the figures. (Also correcting some typos here and there).
   Done ... let me know of remaining typos as they appear

2. I do not understand the plural of "at certain levels" (Fig. 7B). I would expect a fixed N_0 (what value is not important according to Fig. 7A).
   I actually plotted for several N_0 somewhat naively and as it doesn't matter, all curves give exactly the same line. Could be written differently I suppose.

3. We may be able fit the model to Kaissling's data and so determine some of the unknown parameters.
   That would be very good to tie things more to reality. I assume we may be able to get some information on the de- and adsorption rates (or at least their ratio).

4. We may also be able to interpret part (or all) of our recent experiments (which are being analyzed by Marta).
   That would be the idea. hopefully the model is close enough to reality to connect it to experiments.