Pheromone output of a simple olfactometer

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27-03-2008

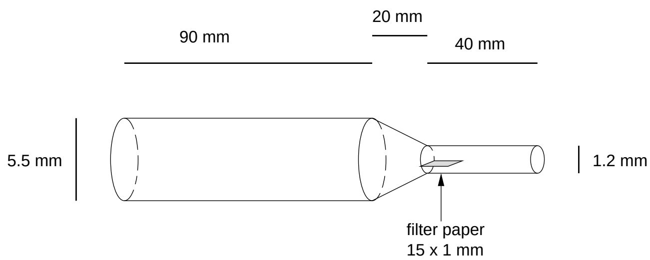

Figure 1: Geometry of the cartouchede stimulation: We assume for simplification that it is cylindrical for most of its length and contracts in a straight line in between. The inside diameters are exact at the ends.

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 isbased on numerical simulations taking an approximate geometry into account (Fig. 1). A realistic geometry could easily be substituted. The results look non-surprising at first until we get to the dpendence of total pheromone output during a puff in dependence on the airspeed in the crtouche de stimulation (see below).

2 Method

The basic geometry for the cartouch 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

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

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

$$+ \frac{A_i}{A_{i+1}\Delta x}kN_{\beta i+1}. \tag{3}$$

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:

$$\frac{dN_{\beta 0}}{dt} = -\Big(\frac{k}{\Delta x} + \frac{v_V}{A_0 \Delta x}\Big) N_{\beta 0} \tag{4}$$

$$+ \frac{A_0}{A_1 \Delta x} \kappa N_{\beta 1}. \tag{5}$$

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

$$\frac{dN_{\beta N-1}}{dt} = -\Big(\frac{A_{N-2}}{A_{N-1}\Delta x}\kappa + \frac{k}{\Delta x} + \frac{v_V}{A_{N-1}\Delta x}\Big) N_{\beta N-1} \tag{6}$$

$$+ \Big(\frac{k}{\Delta x} + \frac{v_V}{A_{N-2}\Delta x}\Big) N_{\beta N-2}. \tag{7}$$

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 conpartments 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, $N_{\alpha i} = N_{\text{pher}}/15$, $i = 0, \ldots, 14$ and no pheromone is in the air, $N_{\beta i} = 0$, $i = 0, \ldots, 149$.

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. The results are illustrated in figures 2 and 3 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 4. 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 5 illustrates the results. Pheromone delivery can be measured as peak delivery rate or as total number of molecules delivered. We show data for both.

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 5A. 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. But we already see a surprise: The dependence on the air speed seems inverted.

This becomes more clear in plot where we fix the number of dpeosited molecules and vary the airspeed of the puff. (Fig. 5B and 6B). From the former figure we deduce that the maximal rate of ejected pheromone is linearly increasing with increasing airspeed. The figure shows the maximum rate normalized by the total number deposited which collapses all 16 curves onto one line.

A completely different picture emerges for the total number of ejected molecules. Here we observe a decline with growing airspeed after an initial rise for very slow speeds. Again we normalized by the total number deposited which approximately collapses the curves

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.

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. 7).

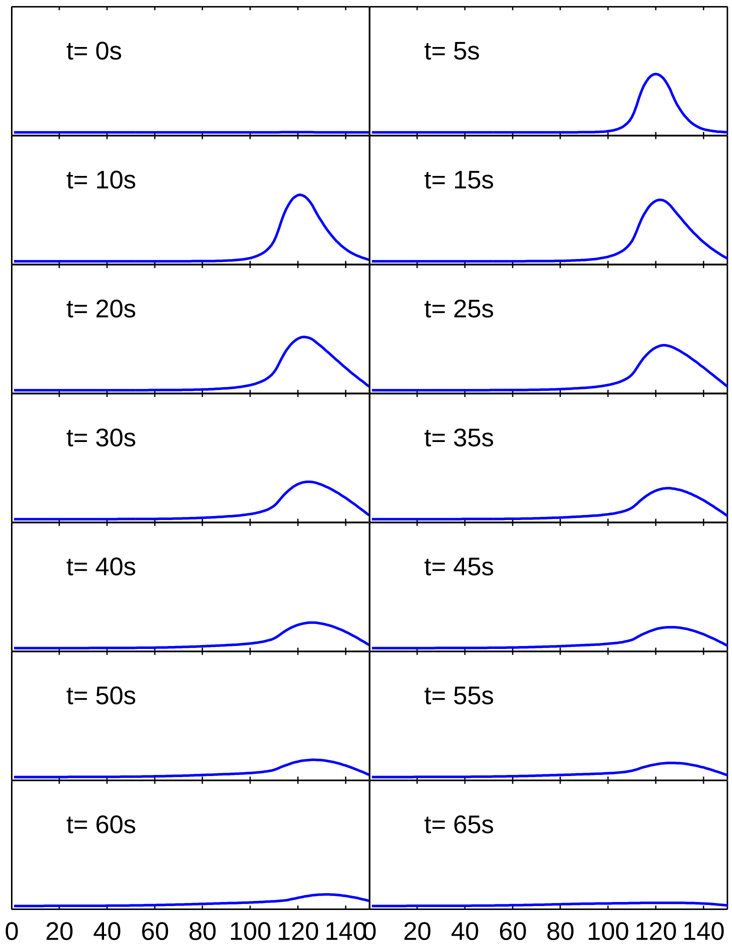

Figure 2: Profiles of pheromone concentration (molecules/m^2) in the cartouche de stimulation over time assuming fairly fast desorption and diffusion. The left end is closed (see equation (5)). The right end is open so that pheromone can leak out but no pheromone comes back in (assumption of an infinite volume outside). The kinks in the shape of the profile are caused by the diameter changes in the pipette according to figure 1.

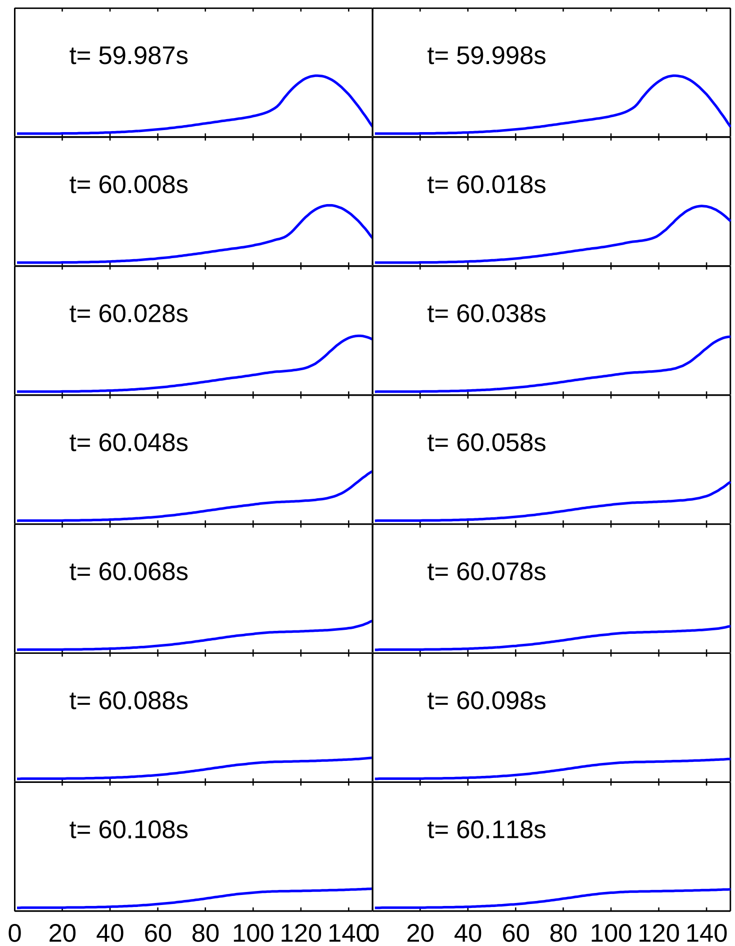

Figure 3: Profiles at the times around the puff. One sees how the concentration profile if just pushed through the pipette to the right. After the puff the pheromone continues to leak out (not shown here).

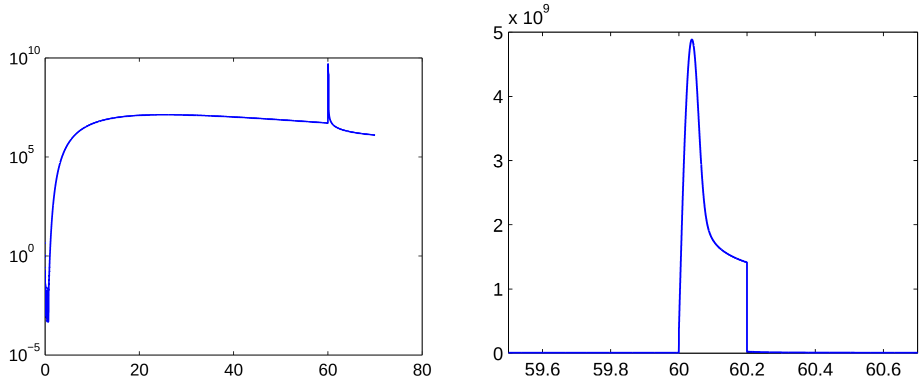

Figure 4: Rate of pheromone exiting the cartouche de stimulation (molecules/s). A) logarithmic plot demonstrating the leakage before and after the puff. B) temporal high resolution picture of the puff itself. Clearly the puf is by no means a square profile.

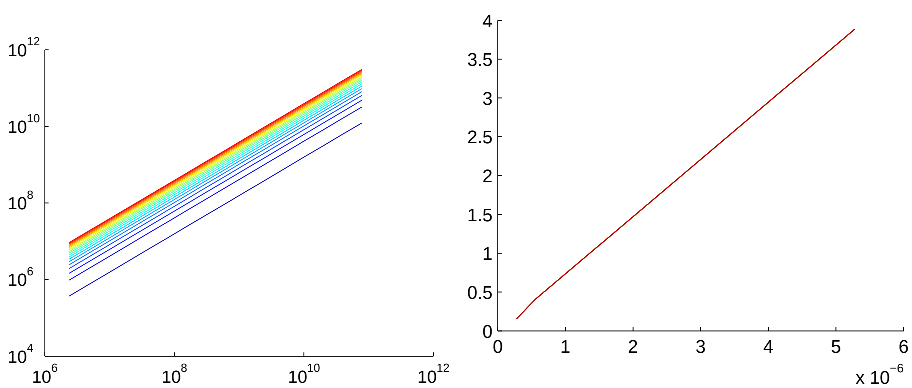

Figure 5: Dependence of the maximal exit rate from the cartouche (which occurs during he puff) in dependence on the number of molecules deposited (A) and for fixed number of deposited molecules in dependence on the air speed of the puff (B).

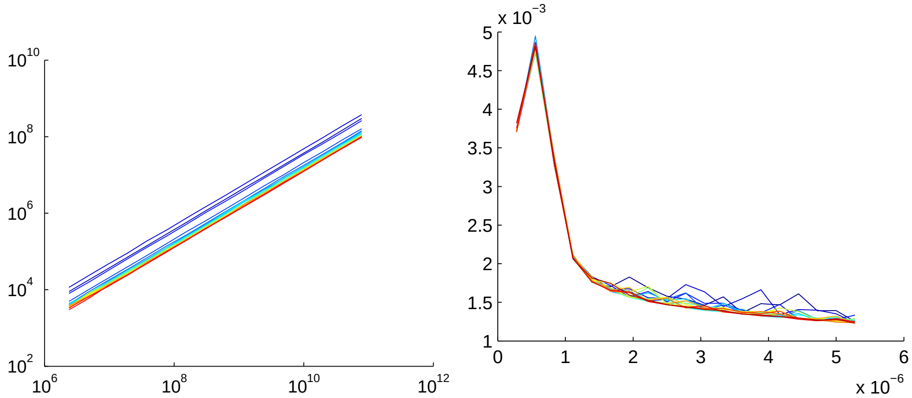

Figure 6: Dependence of the number of pheromone molecules exiting the cartouche during the puff (between 60 s and 60.2 s) in dependence on the number of molecules deposited (A) and for fixed number of deposited molecules in dependence on the air speed of the puff (B).

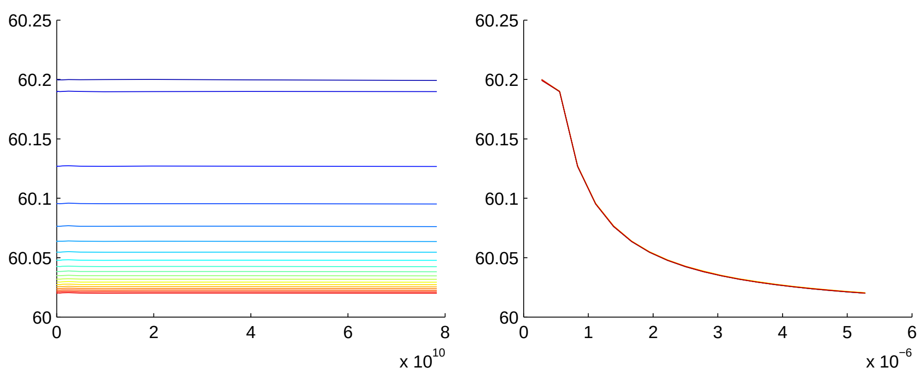

Figure 7: Time of occurence of the maximal rate of molecules exiting the cartouche de stimulation. A) in dpendence on the number of dpeosited molecules at a set of fixed airspeeds and B) as a function of the airspeed at certain levels of deposited pheromone