# Supplementary Material to "Do terrestrial hermit crabs sniff? Air flow and odorant capture by flicking antennules"

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**Abstract**

Supplementary material accompanying the paper "Do terrestrial hermit crabs sniff? Air flow and odorant capture by flicking antennules." Includes details of the computational model simulating odor transport to the chemosensory hairs based on PIV data.

**Keywords**: olfaction, hermit crab, fluid dynamics, aesthetasc, flicking

## Markov-Chain Monte Carlo Computational Model

We simulated the transport of odorant molecules to the ventral surfaces of aesthetascs on an antennule of *C. rugosus*, using a 2D Markov-chain Monte Carlo simulation. To simulate convection during flicks,

we used our PIV data in air with a finite-difference, forward-Euler approximation, and to simulate diffusion, we used two, 1D random walks of odorant molecules. All simulations were performed in Matlab (R2014a). The flick was divided into n time steps with duration $\Delta t = 7.82 \times 10^{-6}$ s. For each time step, the position $P(X, Y)$ of each odour molecule was advanced using a finite-difference, forward Euler approximation based on PIV velocity vector fields:

$$X(t + 1/2\Delta t) = X(t) + u(X(t))\Delta t \tag{1}$$

$$Y(t + 1/2\Delta t) = Y(t) + v(Y(t))\Delta t \tag{2}$$

Eqn. 1 uses $u$ for the $X$ component of position and Eq. 2 uses $v$ for the $Y$ component of position. Diffusion for each time step was advanced based on the root mean squared distance of diffusion ($L_{RMS} = \sqrt{2D\Delta t}$) to yield the equations:

$$X(t + \Delta t) = X(t + 1/2\Delta t) + i\sqrt{D\Delta t} \tag{3}$$

$$Y(t + \Delta t) = Y(t + 1/2\Delta t) + i\sqrt{D\Delta t} \tag{4}$$

where $i$ was assigned the values -1, 0, or +1 based on Matlab's pseudorandom number generator for each component of position independently.

A patch of 100,000 simulated odorant molecules ($M_{total}$) was created over an area of $3.48 \times 10^{-10}$ $m^2$ (see Fig. 1); odorant molecules were evenly spaced along each axis within the area. The density of simulated odorant molecules corresponds to a concentration of 0.46 parts per billion of caproic acid in air based on mass.

We assumed that the aesthetasc array was a perfect absorber, so that any odor molecules that crossed the boundary line were removed from the fluid and counted as captured at each time step. The total number of molecules captured was divided by the starting number of molecules to find the percent total molecules captured, $M$. The location of the outer boundary of the physical model's aesthetasc array was chosen from raw data images (shown in Fig. 1, all panels).

Since we used measured PIV velocity vector fields, there was the possibility that non-zero velocity vectors could exist close to or on the boundary of each aesthetasc due to measurement error, which would be a violation of the no-slip condition. We verified that there was no violation of the no-slip condition by running a simulation in which diffusion coefficient $D$ was set to 0 (no diffusion case); the no-diffusion case captured no molecules during an entire downstroke-return stroke event, indicating that either the no-slip condition is not violated or that the violations were so small that they did not inflate the capture of simulated molecules.

Another assumption of our computational was that the velocity vector field was divergence-free, an indication that there is no flow in the dimension normal to the plan in which we measured velocities. Divergence is relatively low, except at position values very close to the edge of the plot (Fig. 2, high $X$-position values). Since these are 2D velocity vector fields sampled from a 3D velocity vector field, divergence in 2D fields is expected. In other models, 2D velocity vector fields were decomposed to create non-unique solutions of divergence and divergence-free velocity fields which differ from the measured fields [1], but we have chosen to rely on raw PIV data from the model without this decomposition in order to stay true to fluid flow around the model.

## Convergence Testing

To determine the time-step used for simulations, simulations were run using numbers of steps ranging from 100 to 20,000 with 100,000 simulated molecules with $D = 6 \times 10^{-6}$ m$^2$ s$^{-1}$ for three repetitions (Fig. 3A). Convergence on a final number of molecules per total molecules captured was observed at around 8.8%. The number of steps reaching very close (within the standard deviation of three runs) by 10,000 time steps, so this number ($\Delta t = 7.82 \times 10^{-6}$ s) was chosen for all runs with diffusivities.

Convergence in concentration was tested by varying $M_{total}$ within the initial starting area between 2,500 and 12.3 million simulated molecules, corresponding roughly to concentrations of 0.0012 to 5.65 ppb in air (Fig. 3B). Three repetitions of these conditions revealed that the per-cent of total molecules captured had no dependence on initial concentration, but higher standard deviations were observed for concentrations under 0.4615 ppb (100,000 simulated molecules), so a concentration of 0.46 ppb was used for simulations unless otherwise noted.

## Data Archiving

All data are available at FigShare: http://dx.doi.org/10.6084/m9.figshare.1558300.

# References

[1] Stacey, M., Mead, K. & Koehl, M., 2002 Molecule capture by olfactory antennules: Mantis shrimp. *J. Math. Biol.* **44**, 1–30.

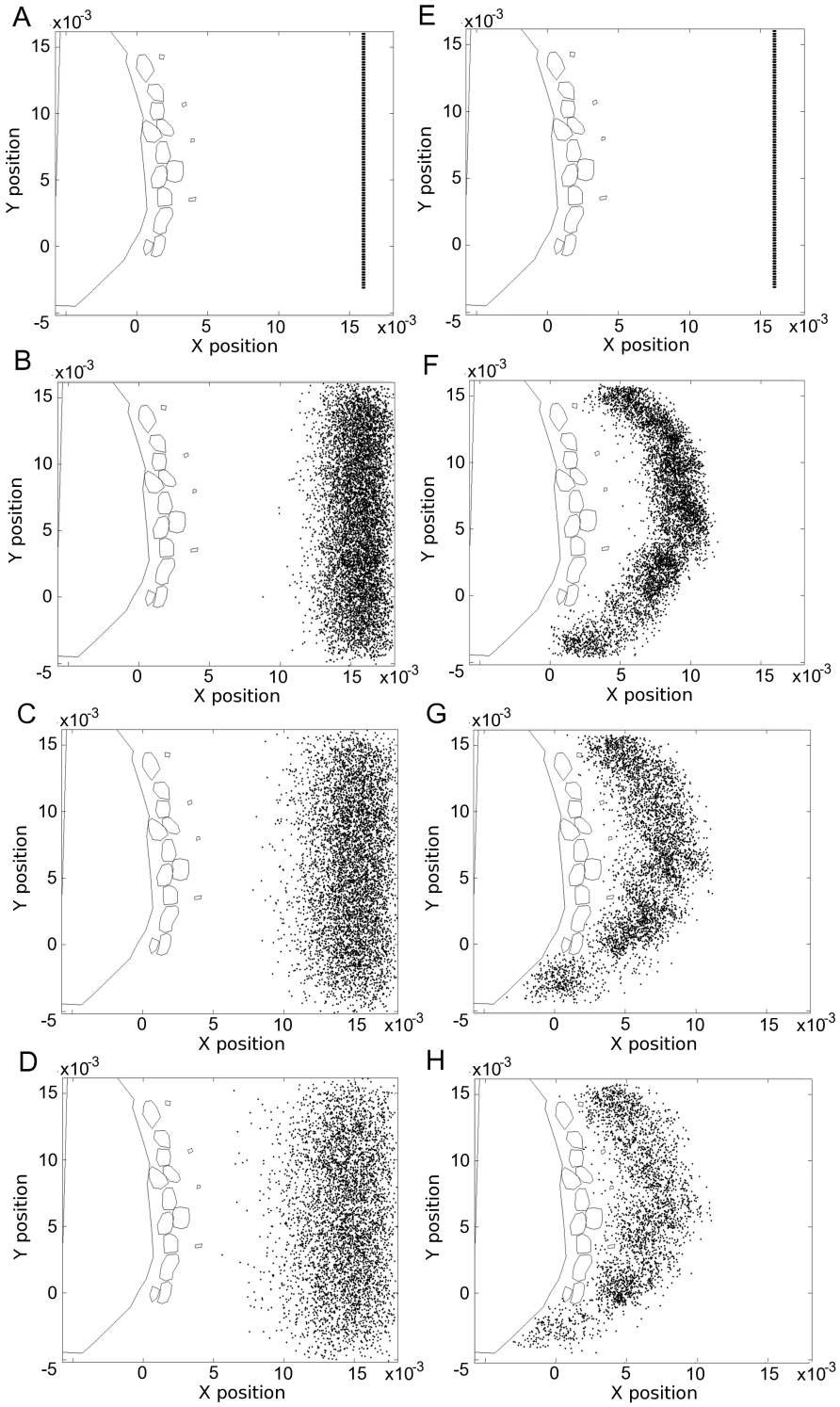
A
E
B
F
C
G
D
H
x10-3
Y position
X position
15
10
5
0
-5
0
5
10
15

Figure 1 *(preceding page)*: Computational model of odor transport based on grid established during particle image velocimetry at $D = 5 \times 10^{-8}$ m$^2$ s$^{-1}$ for two simulation conditions: still antennule (A-D) and flicking antennule (E-H). Position of the flagellum and aesthetascs marked with black lines. The positions of simulated odor molecules are plotted at times 0 s (initial positions; A,E), 7.82 ms (B,F), 15.6 ms (C,G), and 23.5 ms (D,H).

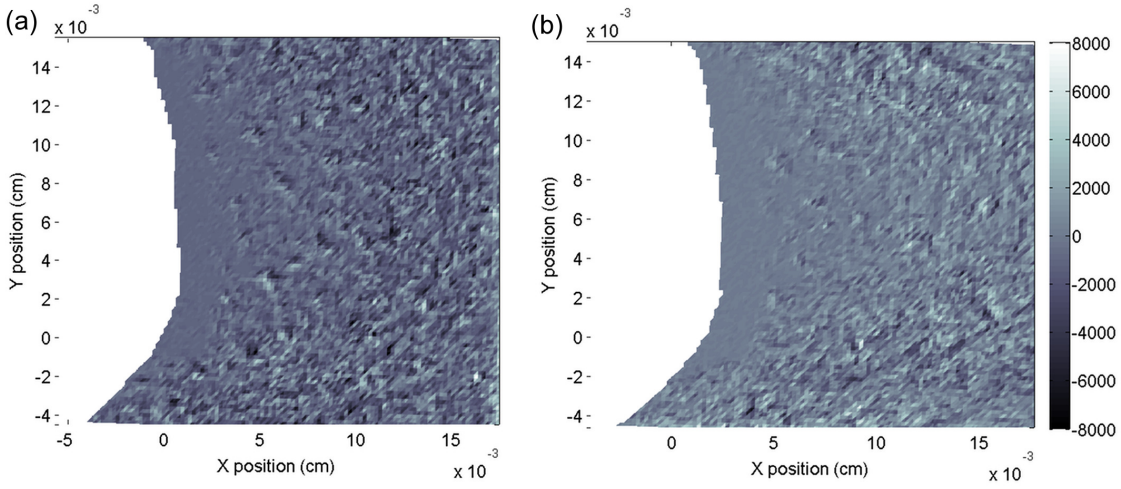


Figure 2: Divergence of the downstroke (a) and return stroke (b) PIV velocity vector fields used for the computational model.

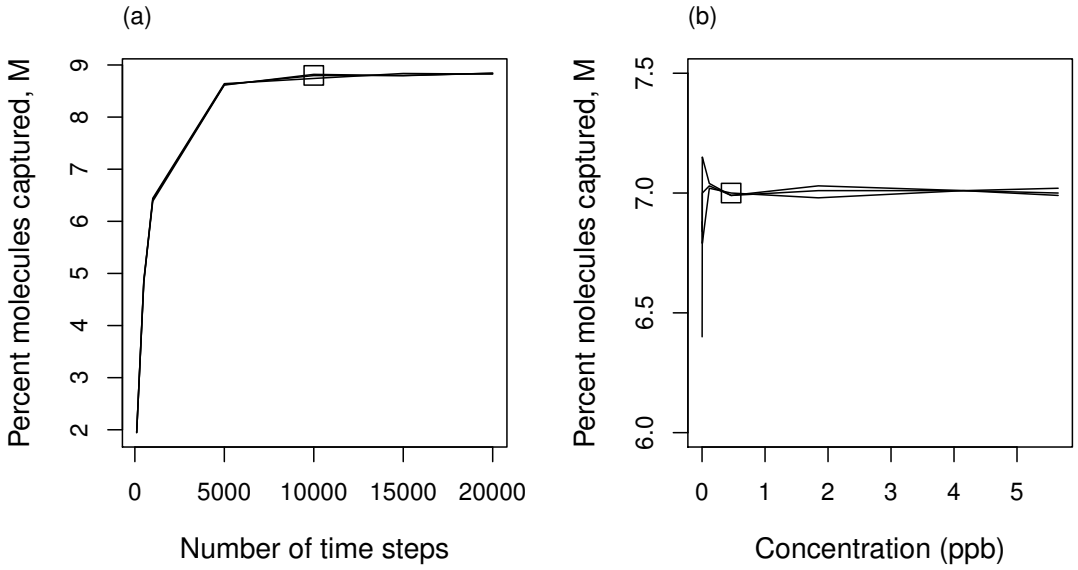


Figure 3: Convergence testing plots for diffusivities in air ($D = 6.02 \times 10^{-6}$ m$^2$ s$^{-1}$). Each plot contains three replicate simulations at each point. Square boxes indicate chosen parameters for regular simulations. A: Temporal. Percentage of total odor molecules captured versus number of time steps that the flick duration was divided. B: Concentration. Percentage of total odor molecules captured versus initial concentration of odor patch in parts per billion (ppb).