Dispersion of solute released from a sphere flowing in a microchannel: Supporting Information

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S1. STOCHASTIC SIMULATIONS

Besides the numerical integration of the axisymmetric Fokker-Planck equation, we conduct stochastic simulations. Here, the trajectory of a single substance molecule is obtained by integrating the molecule's velocity which at time t is given by

$$\mathbf{v}(t) = \mathbf{u}(\mathbf{r}(t)) + \mathbf{w}(t) \tag{S1}$$

where $\mathbf{u}(\mathbf{r}(t))$ is the fluid velocity at the particle position $\mathbf{r}(t)$. The velocity $\mathbf{w}(t)$ is a random velocity which is drawn from a distribution of random numbers with zero mean and a standard deviation $\sigma_v = \sqrt{\frac{2D}{\Delta t}}$ with the time step Δt. The latter relation can be directly obtained from the flucuation-dissipation theorem applied to the overdamped motion of a massless particle. If a molecule hits the sphere surface, the normal component of the incoming velocity is inverted such that the molecule is reflected back into the fluid. If a molecule crosses the cylinder wall, the trajectory stops. The intial position of the particle at $t = 0$ is located on the sphere surface with the prescribed θ_0. The azimuthal position ϕ_0 is chosen randomly between 0 and 2π such that the full 3D Brownian simulations mimick the axisymmetric situation considered by the finite volume scheme in the main text.

All results obtained from the Fokker-Planck equation in the main text have been verified by these stochastic simulations and excellent agreement was found. Some examples are provided in figure S1.

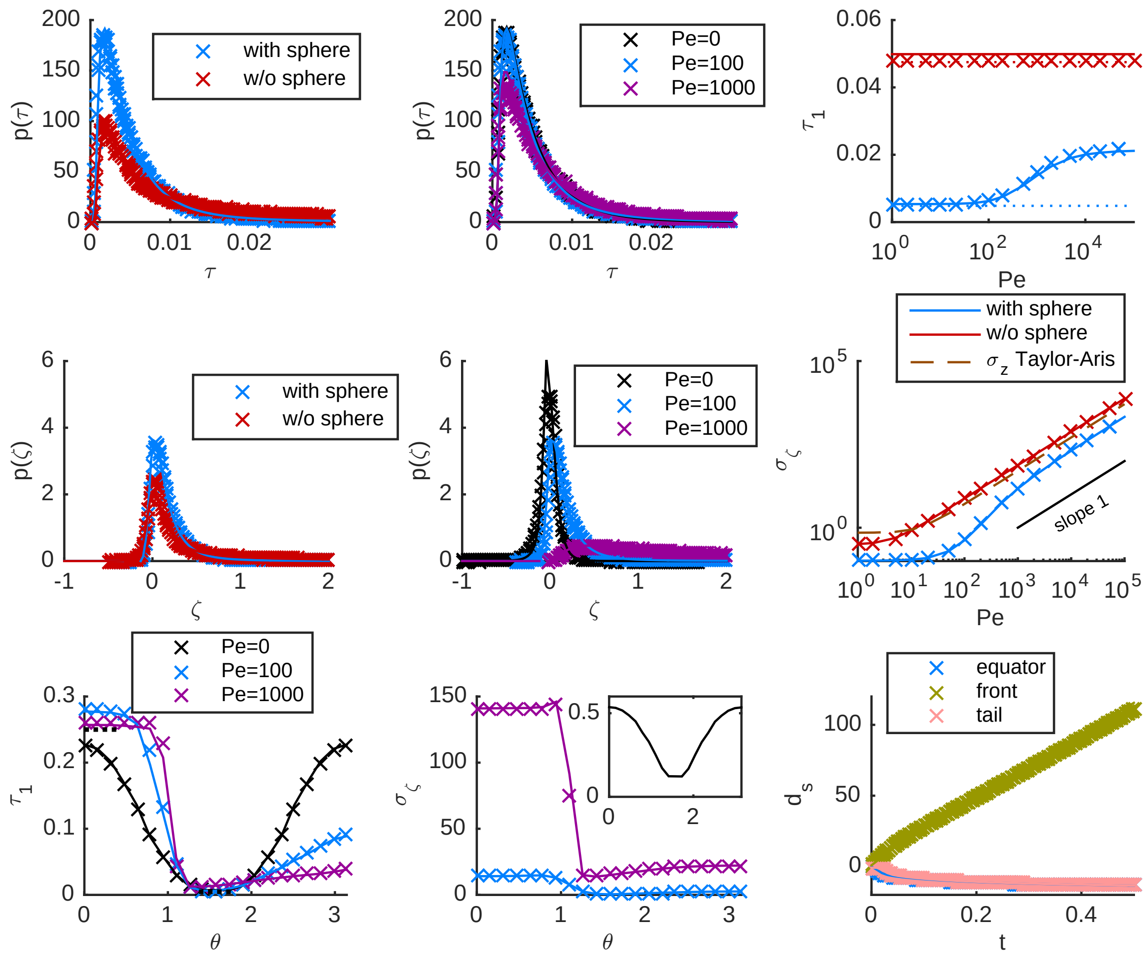

FIG. S1. Analog of figures 2-5 in the main text with lines obtained from the numerical solution of the Fokker-Planck equation and crosses from stochastic simulations.

S2. VARYING SPHERE RADIUS

The analogs of figures 2-7 in the main text for a sphere with radius $R_s = 0.6$ are presented in figure S2. In figure S3 we show in addition the mean residence time and distribution width for $R_s = 0.8$. All aspects mentioned in the main text remain qualitatively similar, although the quantitative influence of the smaller sphere is, of course, less pronounced.

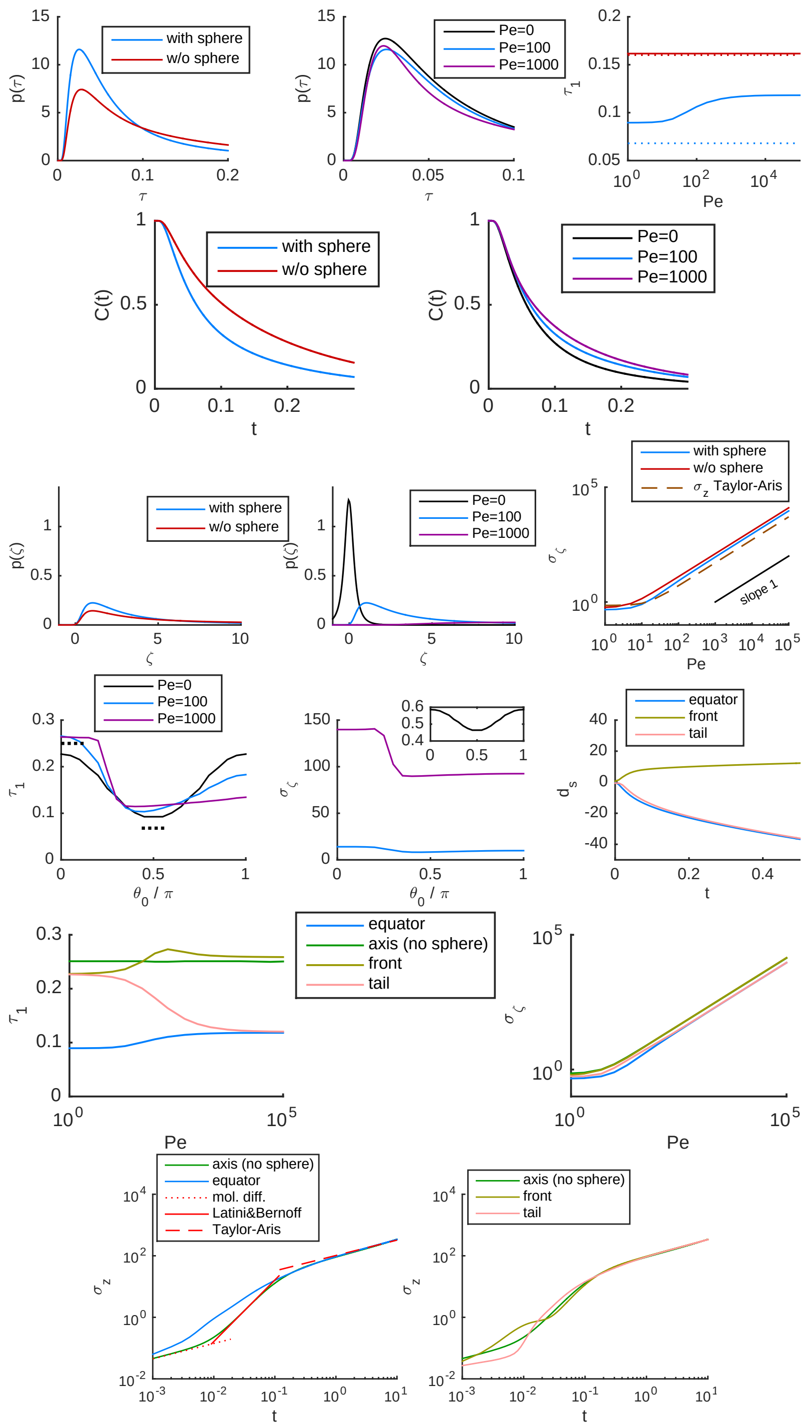

FIG. S2. Data for $R_s = 0.6$

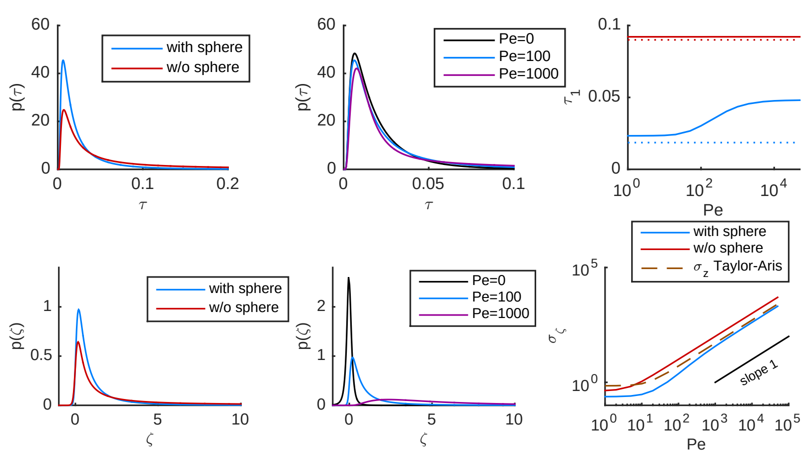

FIG. S3. Data for $R_s = 0.8$