Supporting Information

Single-Walled Carbon Nanotubes Probed with Insulator-based Dielectrophoresis

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This document contains supplementary information describing the numerical model employed in this study, two supplementary movies movies and additional model results for short and long SWNTs.

Numerical model for positive and negative dielectrophoresis trapping of SWNTs:

A numerical model was established with COMSOL 5.2a to study the trapping regions for the positive dielectrophoresis (pDEP) and the negative dielectrophoresis (nDEP) case. A 200 µm long channel with integrated post array was drawn to scale with post diameters of 10 µm and inter-post distances matching those of the experimental device (see main manuscript Figure 1).
The *Electric Current* module was used in a stationary study to compute the electric field distribution in the device. In this module, the electric field distribution was studied by solving the following Maxwell's equations:

$$\nabla . J = Q \tag{1}$$

$$J = \sigma E \tag{2}$$

$$E = -\nabla V \tag{3}$$

Where, J is the current density, E is electric field, V is the potential and Q is the total charge. In the *Electric Currents* model, the posts walls and the side walls of the channel were selected as insulators. An applied potential of 13.3V (scaled according to 1000V applied across the 1.5 cm long microfluidic device) was applied to the inlet boundary and the outlet boundary was grounded. Next, the *Particle Tracing* module was used with a time dependent solver to trace the trajectories of the particles. In this model, the drag force and Brownian force were computed with the following equations:

$$F_D = \frac{1}{\beta} m_p (\vec{u} - \vec{v}) \tag{4}$$

$$\beta = \frac{\rho_p {d_p}^2}{18\mu} \tag{5}$$

$$F_b = \alpha \sqrt{\frac{12\pi k_B \mu T r_p}{\Delta t}} \tag{6}$$

where F_D and F_b are the drag force and Brownian force, m_p, r_p, ρ_p and d_p are the mass, radius, density and diameter of the particle, β is the velocity response time, µ is the viscosity, T is temperature and k_B is the Boltzman constant. u and v are fluid velocity and particle velocity, respectively. Note that the fluid was considered stationary in this study. The dielectrophoretic force $\vec{F}_{dep}$ was also coupled with this model via equation 9 and 10 as described below. With the time dependent solver, the particle trajectories were computed with the following equation:

$$\frac{d(m_p \vec{v})}{dt} = F_t \tag{7}$$

where

$$F_t = F_{dep} + F_D + F_b \tag{8}$$

The DEP force for a spherical particle in a non-uniform electric field can be expressed as:[1]

$$\vec{F}_{dep\_sphere} = 2\pi r_s^3 \varepsilon_m Re(CM) \nabla (\vec{E})^2 \tag{9}$$

where

$$Re(CM) = \frac{\varepsilon_p - \varepsilon_m}{\varepsilon_p + 2\varepsilon_m} \quad (10)$$

Where r_s is the radius of the spherical particle, ε_m is the medium permittivity, ε_p is the particle permittivity and $Re(CM)$ is the real part of the Clausius-Mossotti factor.
COMSOL only allows entries for spherical particles in the *Particle Tracing* module. Therefore, we used an equivalent radius r_{s_eq} for SWNTs assuming that a spherical particle experiences the same DEP force that acts on a rod like SWNT:

$$\vec{F}_{dep\_SWNT} = \vec{F}_{dep\_shpere} \quad (11)$$

where $\vec{F}_{dep\_SWNT}$ corresponds to equation 1 of the main manuscript. Solving for the radius of the sphere renders r_{s_eq}:

$$r_{s\_eq} = \sqrt[3]{\frac{1}{6} * (r_{SWNT}^2 * l)} \quad (12)$$

Where r_{SWNT} and l are the radius and length of SWNTs. We further assume that $Re(CM)$ is the same for the SWNTs and the equivalent spherical particles used in the model and obtain:

$$\varepsilon_{p\_s} = \frac{\varepsilon_m * (1 + 2 * Re(CM))}{1 - Re(CM)} \quad (13)$$

Where ε_{p_s} is the corrected equivalent particle permittivity, entered in the COMSOL model to compute $\vec{F}_{dep\_shpere}$ with the same $Re(CM)$.
In addition, *E* was coupled via the result of the *Electric Current* module altering it with a sine wave function with a frequency of 1000 Hz and corresponding amplitude.
For the pDEP case, r_{SWNT} and l of the SWNTs was used as 0.76 nm and 1000 nm respectively, based on the values obtained through AFM measurements (see main manuscript). With equation (3), r_{s_eq} was found as 5 nm. For the nDEP case, we assumed a r_{SWNT} of 0.76 nm and l of 10 µm considering the shorter sonication time, rendering longer SWNT species. A r_{s_eq} of 10 nm was found and used in the model. According to equation (13), for $Re(CM)$= 18.6 (pDEP) ε_{p_s} resulted in -174.07 and for $Re(CM)$= -0.04 (nDEP), ε_p resulted in 70.94. These values were accordingly entered as model parameters.
The model was solved time dependently for 1000 particles released at the vertical release lines at the middle positions between two rows of posts. Figure 2 of the main manuscript shows the end position after 3 seconds of migration. The supplementary movies show the entire time trace of migration for the 1000 particles released at the vertical release lines in Figure 2.
All parameters used for the numerical model are listed in the Table at the end of this document.

Supplementary Information for the numerical study

Supplementary Video_S1 shows the particle trajectories for the case of **nDEP** for the case shown in the main manuscript Figure 2a, as described above.

Supplementary Video_S2 shows the particle trajectories for the case of **pDEP** for the case shown in the main manuscript Figure 2b, as described above.

Numerical modeling results for non-trapping conditions

We also computed the numerical model for shorter lengths of SWNTs. We considered a length of 100 nm for the pDEP case and 1000 nm length for the nDEP case, which results in r_{s_eq} of 2 nm and 5 nm, respectively. From Figure S1 it can be observed that DEP trapping did not occur in these two cases. The DEP force is not strong enough to trap the particles for these two cases and characteristic trapping regions can not be observed.

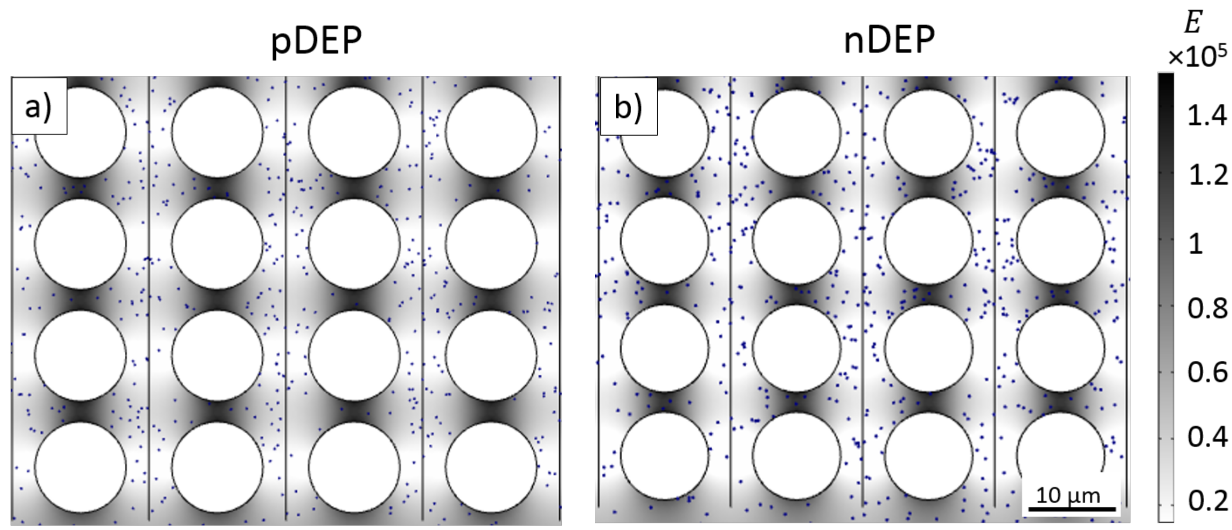

Figure S1: a) Position of SWNT (shown as blue dots) with length of 100 nm predicted with the numerical model for $Re(CM) > 0$. The image shows the end position of 1000 SWNTs released from each vertical line. SWNTs were not trapped by DEP in the post array. b) Similar to a) but for the nDEP case with $Re(CM)<0$. SWNTs of 100 nm length did also not trap in the post array. The grey scale surface plot in a) and b) indicates electric field strength.

Numerical modeling results for trapping conditions (nDEP case only)

We further studied the nDEP case of the SWNTs with the numerical model inducing larger DEP forces. Longer SWNTs of l = 100 µm with r_{SWNT} = 0.76nm were considered and we obtained r_{s_eq} of 21 nm from equation (12). From Figure S2 it can be observed that SWNTs trapped closer to the circular posts compared to Figure 2a of the main manuscript.

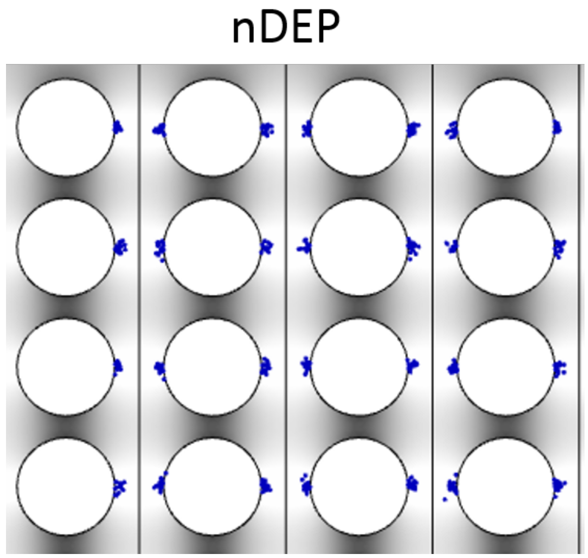

Figure S2: a) SWNT (shown as blue dots) with length of 100μm position predicted with the numerical model for Re(CM)< 0. The image shows the end position of 1000 SWNTs released from each vertical line. SWNTs were trapped by DEP in the post array

Table S1: Parameters used for numerical modeling

Variable	Value	Unit
Applied potential	13.3	V
Temperature	298	K
Density of water	997.0479	kg/m^3
Density of SWNT	1600	kg/m^3
Frequency	1000	Hz
Viscosity of water	0.00089	Pa s
Particle permittivity (ε_{p_s}), for pDEP	-174.07	n.a.
Particle permittivity (ε_{p_s}), for nDEP	70.94	n.a.

References

1. Jones, T. B., *Electromechanics of Particles*. Cambridge University Press: New York, 1995.