Supplementary Information for

Nanofluidic Charged-Coupled Devices for Controlled DNA Transport and Separation

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Model and Simulation Details

The coupled mathematical model consists of PNP equations for both ions and molecules that were numerically solved by COMSOL Multiphysics. The "Electrostatics" and "Transport of Diluted Species" modules were utilized to solve the 2D versions of equations S1-S3:

$$\frac{d^2V(t)}{dx} + \frac{d^2V(t)}{dy} = -eN_A(\sum_i z_i c_i(t)\,)/\varepsilon_0\varepsilon_r \qquad \text{(S1)}$$

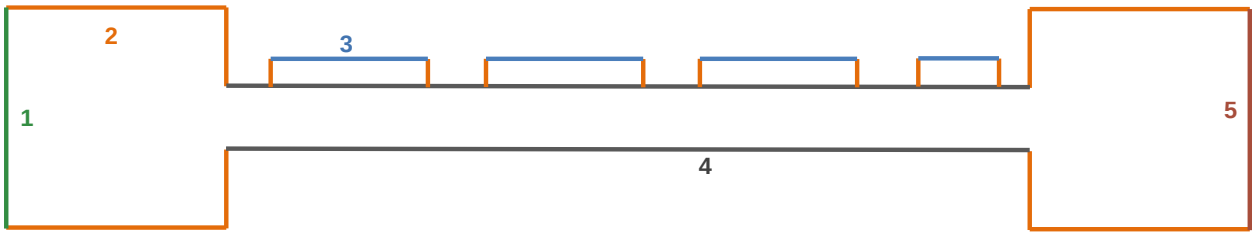
$$\frac{\partial c_i(t)}{\partial t} + \frac{dJ_{ix}(t)}{dx} + \frac{dJ_{iy}(t)}{dx} = 0 \qquad \text{(S2)}$$

$$J_i x(t) = -D_i \frac{dc_i(t)}{dx} - c_i(t)\left(z_i \mu_i \frac{dV(t)}{dx}\right)$$

$$J_i y(t) = -D_i \frac{dc_i(t)}{dy} - c_i(t)\left(z_i \mu_i \frac{dV(t)}{dy}\right) \qquad \text{(S3)}$$

DNA, Cl^-, and K^+ was chosen as the model molecule and ions, respectively, for the required parameters in equations S1-S3 (**Table S1**). The numerical domain was generated based on our design for the CCD device (**Figure S1a**). While the Electrostatics model (Eq.S1) was considered for all sections of the numerical domain (gates, reservoirs, and nanochannel), "Transport of Diluted Species" modules (Eq.S2 and S3) were only solved in the nanochannel and reservoirs. Appropriate boundary conditions were chosen for each set of equations **(Figure S1b).** A higher density of grids were generated in regions with higher variables gradient (*e.g.*, vicinity of channel walls) and *vice versa* (**Figure S2**). The total number of grids for the model with one set of gates are 25941 with an area ratio (ratio between the areas of the largest and smallest element) of 7.2×10^{-4}. The solver's relative tolerance, which is the maximum amount of error that we allowed in our simulations, was 0.0005.

a)



b)

Boundary \ Equation	Poisson's Equation	Transport of Ions and molecules
1	Ground	Zero flux
2	$n \cdot D = 0$	Zero flux
3	$V = V_G(t)$	-
4	$n \cdot (D_1 - D_2) = \sigma_s$	Zero flux
5	$V = V_C$	Zero flux

c)

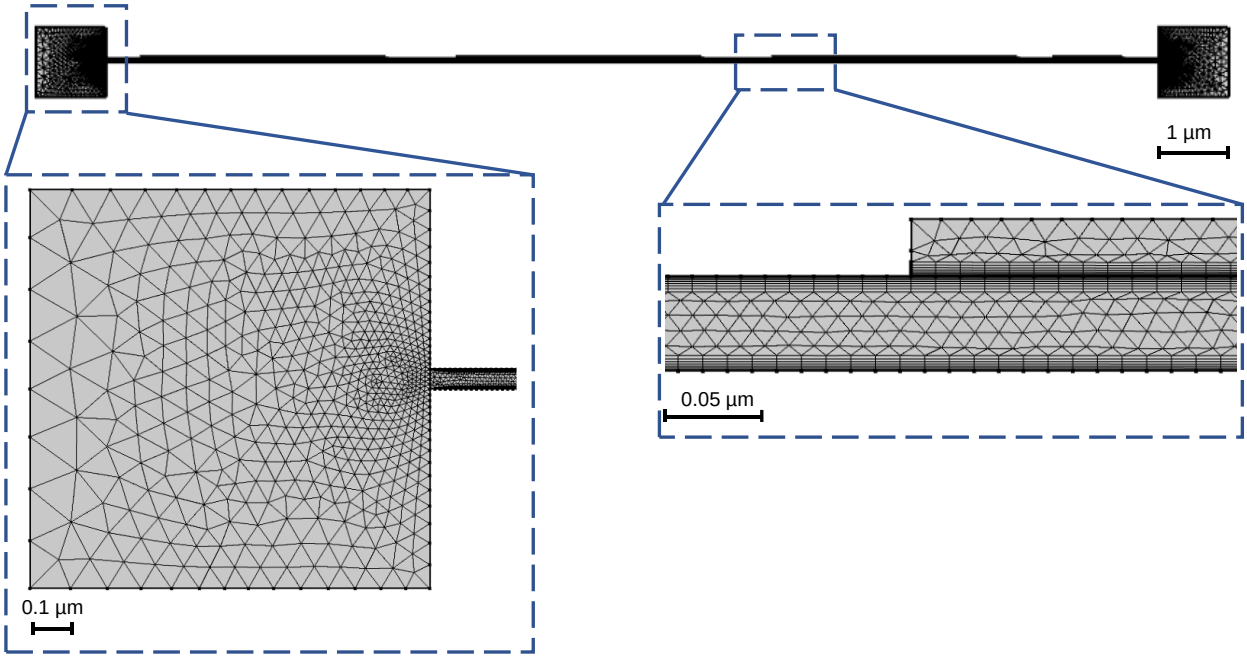


Figure S1. a) A two-dimensional computational domain used for our numerical platform. The reservoir size is 1 µm×1 µm, and the nanochannel width is 50 nm. The gates are 3.5 µm×30 nm in size and are separated by 1 µm gap. b) The boundary condition for each set of equations: Poisson and Nernst-Planck for ions and molecules (DNA). c) Distribution of the grids through the computational domains

Table S1. Summarization of the parameters used in the numerical simulation.

Parameter	Meaning	Value	Unit
e	Elementary charge	1.6×10^{-19}	C
ε_0	Vacuum permittivity	8.85×10^{-12}	C/Vm
ε_{r1}	Relative permittivity	70	1
ε_{r2}	Relative permittivity	5	1
σ	Surface charge density	-2×10^{-3}	$\mathrm{C/m^2}$
V_c	Bias Voltage	0.4	V
C_{ion}	ions concentration	1	$\mathrm{mol/m^3}$
T	Temperature	300	K
D_{Cl^-}	Diffusivity of Cl^-	2.03×10^{-9}	m^2/s
D_{K^+}	Diffusivity of K^+	1.96×10^{-9}	m^2/s
D_{DNA}	Diffusivity of DNA	2.1×10^{-12}	m^2/s
μ_{Cl}	Electrophoretic mobility of Cl^-	7.85×10^{-8}	m^2/Vs
μ_K	Electrophoretic mobility of K^+	7.58×10^{-8}	m^2/Vs
μ_{DNA}	Electrophoretic mobility of DNA	4.3×10^{-8}	m^2/Vs
η	Transport eficciency	Variable	1
RA	Relative abundance	Variable	1