Electronic Supplementary Information (ESI)

Effects of access resistance on the resistive pulse caused by a translocating

nanoparticle through a nanopore

Junrong Wang,[1] Jian Ma,[2] Zhonghua Ni,[2] Li Zhang[3] and Guoqing Hu[1]*

[1] Institute of Mechanics, Chinese Academy of Sciences, Beijing 100190, China
[2] Jiangsu Key Laboratory for Design and Manufacture of Micro-Nano Biomedical Instruments, Southeast University, Nanjing 211189, China
[3] Research and Development Center, Synfuels China Technology Co., Ltd., Beijing 101407, China

* Corresponding author: guoqing.hu@imech.ac.cn

1. Mathematical model implementation

Fig. S1 shows the schematic view of the axisymmetric nanopore Coulter counter system in our simulation. Taking advantage of axi-symmetry, a two-dimensional cylindrical coordinate system (r, z) can be adopted for more efficient simulations.
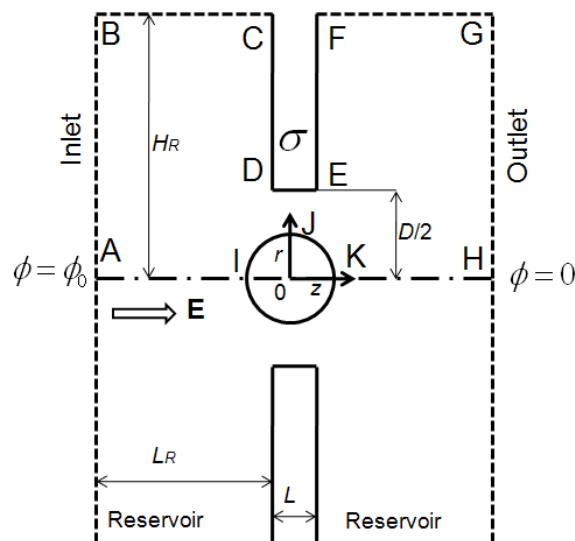
Fig. S1. A schematic depiction of the computational domain used in this study.

1.1 The Laplace model

It is convenient to normalize the Laplace model. We use the applied voltage ϕ_0 as the potential scale, the pore's diameter D as the length scale. The dimensionless equation of the Laplace model becomes

$$\nabla^2 \Phi = 0 \tag{R1}$$

with the boundary conditions

Inlet (AB): $\Phi = 1$ (R2)

Outlet (GH): $\Phi = 0$ (R3)

All walls: $\mathbf{n} \cdot \nabla \Phi = 0$ (R4)

where $\mathbf{n}$ is the unit outer normal vector.

In our simulations, the reservoirs are assumed to be infinite. A nanopore system with lower thickness-to-diameter aspect ratios (L/D) has larger reservoirs in our computation. Fig. S2 shows the variation of the resistive-pulse amplitude as a function of the scaled reservoirs length (L_R/D) for the nanopore system with $D = 5L$.
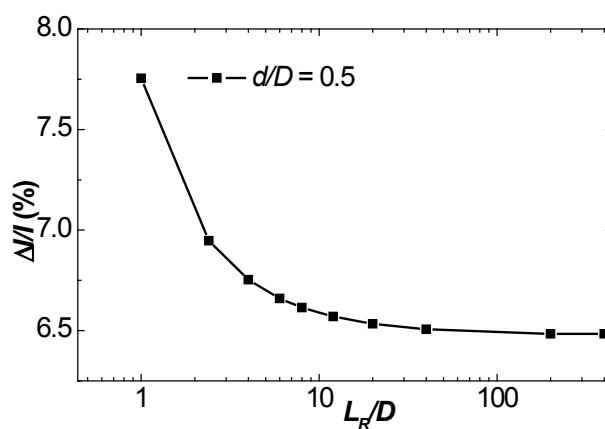
Fig. S2. The resistive-pulse amplitude varies as a function of the scaled reservoirs length (L_R/D) for nanopore system with $D = 5L$.

A typical reservoir size for our computation of the $D = 5L = 250$ nm nanopore system is $L_R = 5$ μm and $H_R = 10$ μm. Since the two reservoirs are assumed to be infinitely large, for a given particle-nanopore system with the same L/D and d/D ratios, we will always get the same $\Delta I/I$.

1.2 The PNP-NS model

The nanoparticle translational velocity, $\mathbf{u}_p = U_p \mathbf{e}_z$, is an important parameter for boundary conditions of the PNP-NS model. However, it is unknown a priori and needs to be calculated by satisfying the z component force balance on the particle:[1, 2]

$F_E + F_D = 0$ (R5)

Here, F_E and F_D are, respectively, the electrostatic and hydrodynamic drag

forces in the z direction:

$$F_E = \iint_S \sigma_p \cdot (-\partial\phi / \partial z) dS \qquad (R6)$$

and

$$F_D = -\iint_S \left[\mu(\partial u_z / \partial r + \partial u_r / \partial z) \cdot n_r + (2\mu\partial u_z / \partial z - p) \cdot n_z \right] dS \qquad (R7)$$

where S is the surface of the particle, and n_r and n_z are, respectively, the r and z components of the unit vector $\mathbf{n}$.

The solution process for the particle's velocity is as follows: (i) calculate the PNP-NS equations with an initial value (e.g., $U_p = 0$) of the particle's velocity; (ii) update U_p using the Newton–Raphson method until the total forces were balanced. Usually, it takes less than five iterative steps for convergence.

In this study, we consider KCl aqueous solution filled in the nanopore system. The relative permittivity of KCl aqueous solution is $\varepsilon_r = 80$, the diffusivities of K$^+$ and Cl$^-$, D_{K^+} and D_{Cl^-}, are 1.957×10^{-9} m^2/s and 2.032×10^{-9} m^2/s, respectively, the fluid density is $\rho = 1000$ kg/m^3; the fluid viscosity is $\mu = 1\times10^{-3}$ Pa·s, the temperature is $T = 300$ K, and the applied voltage is $\phi_0 = 0.1\ V$.

2. Numerical results for other uncharged nanopore systems

Besides the two typical nanopore system with $D = L$ and $D = 5L$ in the text, we have also calculated various nanopore systems with D/L ranging from 0.1 to 10. Fig. S3 displays comparisons of the numerical results with different analytic predictions on resistive-pulse amplitude caused by a particle ($d/D = 0.5$) in other nanopore systems. Here, our analytical model for nanopore system with $D \leq L$ is the eqn (13) and eqn (14) with $\beta = 0.5$, and for nanopore system with $D > L$ is the eqn (15) and eqn (14) with $\beta = 0.8$. It can be found that our analytical model agrees very well with numerical results for nanopore systems with $D \leq L$. And for nanopore systems with $D > L$, our analytical model provides better agreement with the numerical results than other models for particles with $d/D \geq 0.4$.
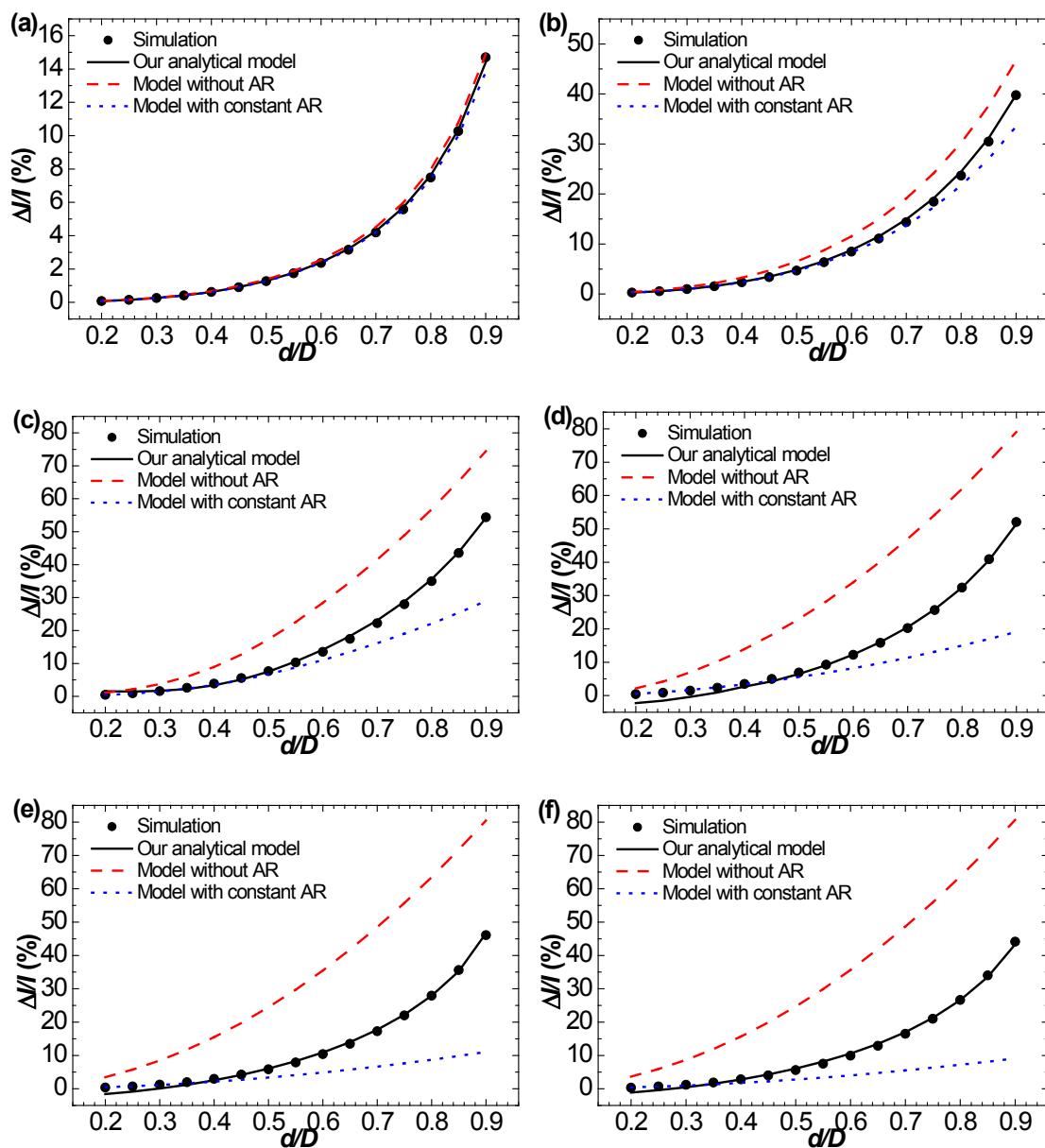
Fig. S3. Comparisons of the numerical results and different analytic predictions on resistive-pulse amplitude caused by a particle with different sizes in a nanopore system with (a) $D/L = 0.1$ (b) $D/L = 0.5$ (c) $D/L = 2$ (d) $D/L = 4$ (e) $D/L = 8$ (f) $D/L = 10$. Our analytical model in (a) and (b) is eqn (13) and eqn (14) with $\beta = 0.5$, and in (c)~(f) is eqn (15) and eqn (14) with $\beta = 0.8$.

1.   S. Qian, A. Wang and J. K. Afonien, *Journal of Colloid and Interface Science*, 2006, **303**, 579-592.

2.   L. H. Yeh, M. K. Zhang, S. Z. Qian and J. P. Hsu, *Nanoscale*, 2012, **4**, 2685-2693.