Article

Supplementary Materials: Translocation of Charged Polymers through a Nanopore in Monovalent and Divalent Salt Solutions: A Scaling Study Exploring over the Entire Driving Force Regimes

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1. Converting the experimental data into the simulation units

In our simulations, the length unit, time unit, and electric field strength unit are, respectively,

$$\begin{aligned} \sigma &= \lambda_B/3.0 \simeq 2.38\times10^{-10}\,\mathrm{m} \simeq 0.7\,\mathrm{bp} \\ t_u &= \sigma\sqrt{m/k_BT} \simeq 2.13\times10^{-12}\,\mathrm{s} \\ E_u &= k_BT/(e\sigma) \simeq 100\,\mathrm{mV/nm} \end{aligned}$$

The explanation, how to obtain these values, can be found in Ref. [1].

Followings are the translocation time reported in five experimental papers. The data converted with our simulation units are given behind the symbol ' $\Longrightarrow$ '.

(1) Experiment by Uplinger et al. [2]:

- molecules: circular supercoiled DNA (pBR322) of ~4.4 kbp $\Longrightarrow$ $N = 6286$
- pore diameter: ~14 nm
- transmembrane field: $E = 120\,\mathrm{mV}/\,15\,\mathrm{nm} = 8\,\mathrm{mV/nm}$ $\Longrightarrow$ $E = 0.08$
- translocation time:
  - (i) $\tau \simeq 110\,\mu$s in 1.6 M KCl solution $\Longrightarrow$ $\tau = 5.16\times10^7$
  - (ii) $\tau \simeq 145\,\mu$s in 1.6 M KCl + 100 mM $MgCl_2$ solution $\Longrightarrow$ $\tau = 6.81\times10^7$

(2) Experiment by Zhang et al. [3]:

- molecules: λ-dsDNA, linear, ~48.5 kbp long $\Longrightarrow$ $N = 69286$
- pore diameter: ~20 nm
- transmembrane field: $E = 600\,\mathrm{mV}/\,20\,\mathrm{nm} = 30\,\mathrm{mV/nm}$ $\Longrightarrow$ $E = 0.3$
- translocation time:
  - (i) $\tau \simeq 0.38$ ms in 1 M KCl solution $\Longrightarrow$ $\tau = 1.78\times10^8$
  - (ii) $\tau \simeq 1.31$ ms in 1 M $MgCl_2$ solution $\Longrightarrow$ $\tau = 6.15\times10^8$

(3) Experiment by Kowalczyk et al. [4]:

- molecules: λ-dsDNA, linear, ~48.5 kbp long $\Longrightarrow$ $N = 69286$
- pore diameter: ~15.3 nm
- transmembrane field: $E = 120\,\mathrm{mV}/\,20\,\mathrm{nm} = 6\,\mathrm{mV/nm}$ $\Longrightarrow$ $E = 0.06$
- translocation time:
  - (i) $\tau \simeq 1.72$ ms in 1 M KCl solution $\Longrightarrow$ $\tau = 8.08\times10^8$
  - (ii) $\tau \simeq 2.94$ ms in 1 M NaCl solution $\Longrightarrow$ $\tau = 1.38\times10^9$

(iii) $\tau \simeq 8.23\,\text{ms}$ in 1 M LiCl solution $\implies \tau = 3.86 \times 10^9$

(4) Experiment by Krueger et al. [5]:

- DNA molecules: circular plasmid pTYB21, 7514 bp long $\implies N = 10734$
- pore diameter: ~20 nm
- transmembrane field: $E = 100\,\text{mV}/\,20\,\text{nm} = 5\,\text{mV/nm}$ $\implies E = 0.05$
- translocation time: $\tau \simeq 300\,\mu\text{s}$ in 1 M KCl solution $\implies \tau = 1.41 \times 10^8$

(5) Experiment by Ito et al. [6]:

- molecules: 9.6 kbp DNA, linear $\implies N = 13714$
- pore diameter: $10 - 25\,\text{nm}$
- transmembrane field: $E = 300\,\text{mV}/\,15\,\text{nm} = 20\,\text{mV/nm}$ $\implies E = 0.2$
- translocation time:

(i) $\tau \simeq 110\,\mu\text{s}$ in 1 M KCl solution $\implies \tau = 5.16 \times 10^7$
(ii) $\tau \simeq 130\,\mu\text{s}$ in 1 M NaCl solution $\implies \tau = 6.10 \times 10^7$
(iii) $\tau \simeq 210\,\mu\text{s}$ in 1 M LiCl solution $\implies \tau = 9.86 \times 10^7$

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