Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.


# Probing of Molecular Replication and Accumulation in Shallow Heat Gradients through Numerical Simulations

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Electronic Supplementary Information (ESI)

# Supplementary Figures

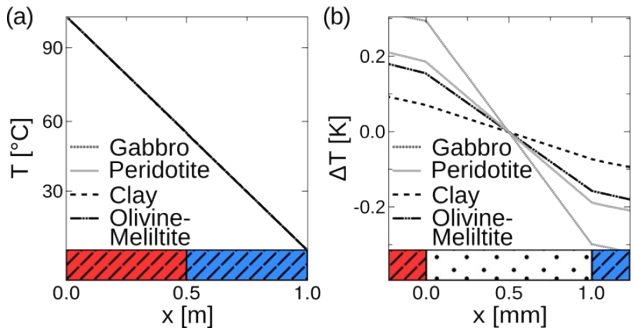


**Fig. S1** Heat flux across porous rocks of various volcanic materials (a) A shallow temperature gradient (0.1 K/mm) is spanned across the porous rock by applying temperatures of 104°C and 4°C to the left and right boundaries, respectively. (b) Steeper temperature gradients emerge across single pores within the porous rock. The focusing of temperature gradient solely depends on the thermal conductivity of the porous rock. Olivine-melilitite for example locally triples the temperature gradient across the pore while gabbro increases the temperature gradient by a factor of six. Hatched areas mark the rocky material and dotted parts represent the water-filled pore.

## Electronic Supplementary Information (ESI)

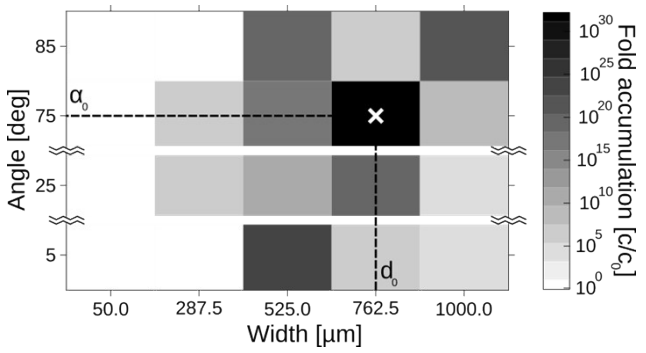


**Fig. S2** Accumulation of 100 mer oligonucleotides with respect to various widths and angles. Each molecule has a distinct accumulation efficiency for a given angle α and width d of the pore. A molecule is defined by its diffusion coefficient D and Soret-coefficient $S_T$, given by $D = 127\ \mu m^2/s$ and $S_T = 0.065\ 1/K$ for a 100 mer oligonucelotide in the warm (70°C) and low salt scenario. The highest accumulation efficiency for a 100 mer is calculated for an angle of $\alpha_0 = 75°$ and width of $d_0 = 762.5\ \mu m$. This method determines the maximum accumulation for each diffusion- and Soret-coefficient displayed in Fig. 4.

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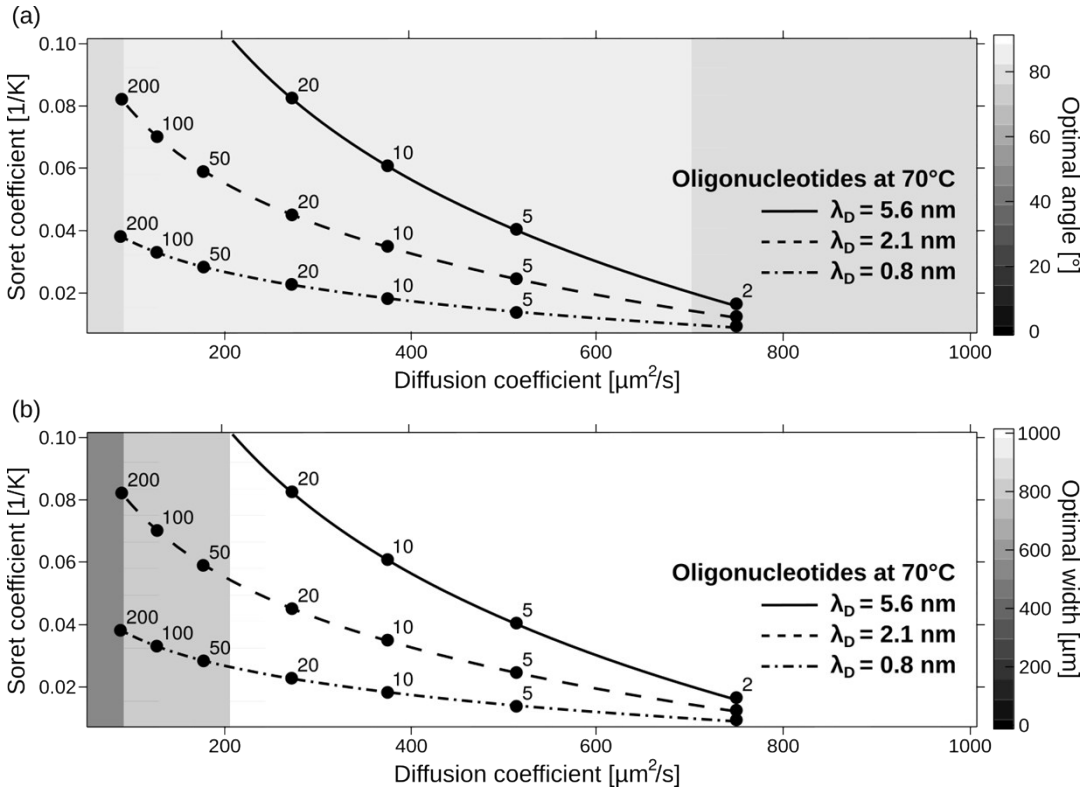


**Fig. S3** Optimal angles and widths for various diffusion coefficients D and Soret-coefficients $S_T$. Accumulation efficiencies are calculated for a given angle α and width d. (a, b) The simulation covers for tilting angles of α = 0°, 25°, 75°, and 85° and widths of d = 50 µm, 287.5 µm, 525 µm, 762.5 µm, and 1000 µm, depicting the angle α and width d with the highest accumulation efficiency. Here, 0° and 90° denote a horizontal and vertical pore, respectively. The diffusion- and Soret-coefficients are screened over 25 uniformly distributed values in the range of 20 µm²/s to 1000 µm²/s and 0.0005 1/K to 0.1 1/K, respectively.

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# Supplementary Files

**Accumulation_Comsol.mph** Sample COMSOL-file set up to determine accumulation efficiencies within pores. Here, heat flux, laminar flow, and concentration for a molecule with $S_T = 0.075$ 1/K and $D = 714$ µm²/s are exemplarily calculated within a rectangular pore with width d = 1 mm, height h = 50 mm, $T_{low} = 55$°C, $T_{high} = 55.5$°C, and a tilting angle $\alpha = 5$°.