SUPPLEMENTARY INFORMATION FOR: Kinetic model of gas transport in carbon nanotube channels

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Transport of two gases through a carbon nanotube channel.

Consider transport of a mixture of two gases through the same carbon nanotube channel where one gas (gas1) has negligible affinity to the nanotube walls and the second gas (gas 2) is able to adsorb on the wall. This situation most closely approximates the case where a gas contains an impurity that has high affinity to the nanotube walls. As described in the main text, the molecules of gas 2 adsorbed on the channel walls change the effective diffusion coefficient for the molecules of gas 1. Thus, if n_1 and n_2 are the concentrations of gas 1 and gas 2, respectively, then the diffusion of gas 1 obeys the Fick's law:

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$$N_1 = -\pi a^2 D(x) \frac{dn_1}{dx} \tag{1}$$

$$D(x) = \frac{1}{3} \bar{v}_1 \frac{d + 2a\alpha n_2(x)}{1 + \alpha n_2(x)} \tag{2}$$

where N_1 is the stationary flux of gas 1. This differential equation has a straightforward solution giving the concentration profile $n1(x)$ and the flux N_1 as:

$$n_1 = n_1^0 \left[1 - \frac{\int\limits_0^x \frac{1+\alpha n_2(x)}{d+2a\alpha n_2(x)} dx}{\int\limits_0^l \frac{1+\alpha n_2(x)}{d+2a\alpha n_2(x)} dx} \right] \tag{3}$$

$$N_1 = \frac{\pi a^2 n_1^0}{3} \sqrt{\frac{8kT}{\pi m_1}} \left[\int\limits_0^l \frac{1 + \alpha n_2(x)}{d + 2a\alpha n_2(x)} dx \right]^{-1} \tag{4}$$

where the concentration profile of gas 2, $n_2(x)$, can be calculated from Eq. 8 (main text). We can use these equations to calculate the reduction in the flux of gas 1 due to the presence of the impurity (gas 2) that interacts with the pore walls (Fig. SFigure 1). Note that even a small fraction of a highly adsorbing gas very quickly "poisons" the transport and sharply reduces the flux of the ideal gas, highlighting the importance of keeping the nanotube pore walls clean for achieving maximum transport efficiency.

Langmuir constant for CH_4 adsorption in carbon nanotubes

To obtain the value of the Langmuir coefficient, α, for adsorption of methane in carbon nanotube we fitted the calculated adsorption isotherm from[1] to the Langmuir equation:

$$A(n) = A_{max} \cdot \frac{\alpha n}{1 + \alpha n} \tag{5}$$

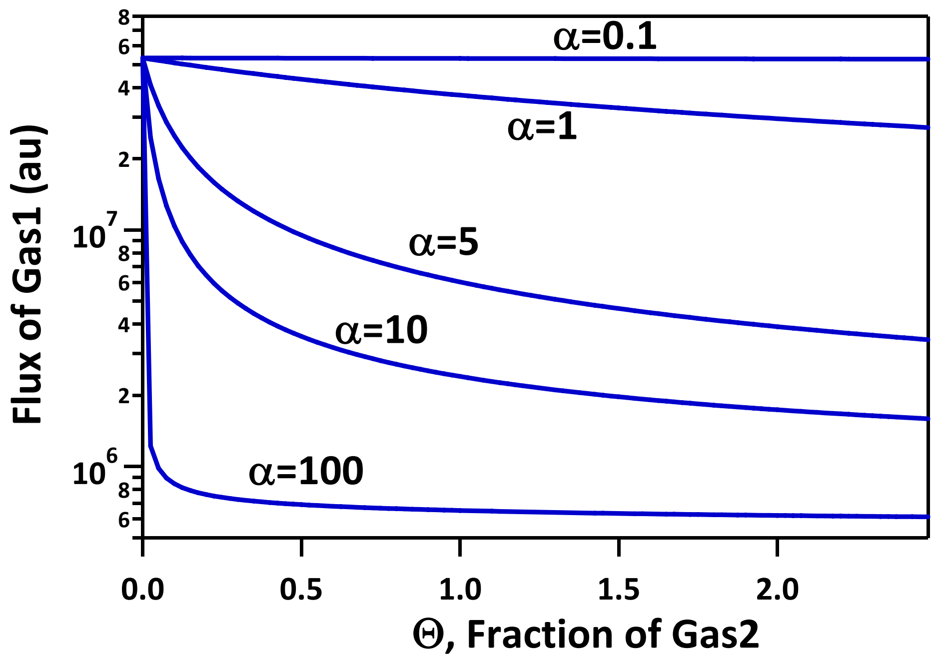

Figure 1: Flux of the ideal gas (Gas1) as a function of the fraction of real gas (Gas2) in the mixture at different values of Langmuir constant α. The concentration of Gas 1 is kept constant. The parameters used for the calculation were: a=0.8nm, d=160nm, l=3000 nm

The fit (Fig. S2) shows reasonably good fit with a value of the Langmuir constant $\alpha = 8.92\text{nm}^3$ (0.217 bar^{-1}).

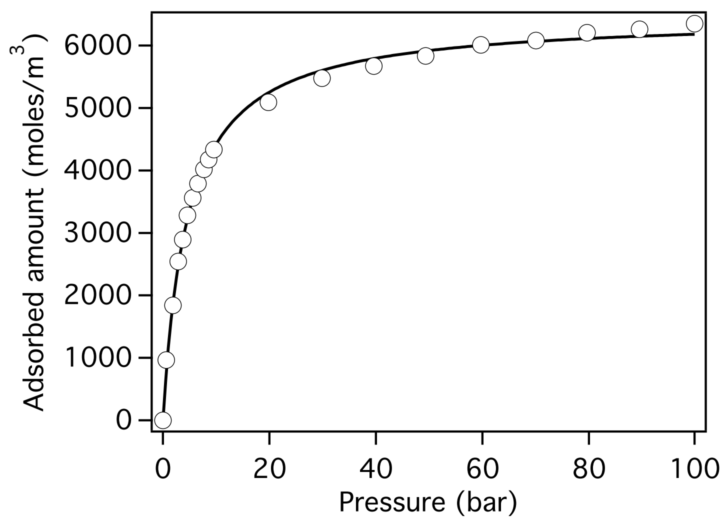

Figure 2: Calculated CH_4 adsorption isotherm in carbon nanotubes fitted to the Langmuir isotherm profile.

References

(1) A. I. Skoulidas, *et. al.* Phys. Rev. Lett. **89**, 185901 (2002).