

Supplementary Information

The origin of a large apparent tortuosity factor for Knudsen diffusion in a samaria aerogel catalyst: a diffusion NMR study

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Table S1. Data used in the least-squares regression to Eq. 4 and the resulting values of D_p model.

p kPa	D_{g0} $\text{m}^2\text{s}^{-1} (\times 10^{-5})$	D_{K0} $\text{m}^2\text{s}^{-1} (\times 10^{-5})$	D_{intra} $\text{m}^2\text{s}^{-1} (\times 10^{-5})$	D_p model $\text{m}^2\text{s}^{-1} (\times 10^{-5})$
10	$13. \pm 2$	0.94	0.15 ± 0.03	0.14 ± 0.04
30	4.0 ± 0.8	0.94	0.14 ± 0.03	0.14 ± 0.05
91	1.5 ± 0.3	0.94	0.12 ± 0.02	0.12 ± 0.03
310	0.4 ± 0.08	0.94	0.079 ± 0.02	0.087 ± 0.03
1000	0.12 ± 0.02	0.94	0.048 ± 0.01	0.044 ± 0.01

Table S2. Data used in the least-squares regression to Eq. 9 and the resulting values of $D_{intra\ model}$.

ρ kPa	D_{g0} $m^2s^{-1} (x 10^{-5})$	D_{K0} $m^2s^{-1} (x 10^{-5})$	$(1-\rho_{surf})$	D_{intra} $m^2s^{-1} (x 10^{-5})$	$D_{intra\ model}$ $m^2s^{-1} (x 10^{-5})$
10	$13. \pm 2$	0.94	0.28 ± 0.06	0.15 ± 0.03	0.13 ± 0.04
30	4.0 ± 0.8	0.94	0.41 ± 0.09	0.14 ± 0.03	0.17 ± 0.05
91	1.5 ± 0.3	0.94	0.35 ± 0.07	0.12 ± 0.02	0.11 ± 0.03
310	0.4 ± 0.08	0.94	0.38 ± 0.08	0.079 ± 0.02	0.066 ± 0.02
1000	0.12 ± 0.02	0.94	0.75 ± 0.15	0.048 ± 0.01	0.052 ± 0.02

Table S3. Data used in the least-squares regression to the modified Eq. 9 where $\eta_K = \eta_g \equiv \eta$ and the resulting values of $D_{intra\ model}$.

ρ kPa	D_{g0} $m^2s^{-1} (x 10^{-5})$	D_{K0} $m^2s^{-1} (x 10^{-5})$	$(1-\rho_{surf})$	D_{intra} $m^2s^{-1} (x 10^{-5})$	$D_{intra\ model}$ $m^2s^{-1} (x 10^{-5})$
10.	$13. \pm 2$	0.94	0.28 ± 0.06	0.15 ± 0.03	0.14 ± 0.04
30.	4.0 ± 0.8	0.94	0.41 ± 0.09	0.14 ± 0.03	0.18 ± 0.05
91.	1.5 ± 0.3	0.94	0.35 ± 0.07	0.12 ± 0.02	0.11 ± 0.03
310 ± 50	0.4 ± 0.08	0.94	0.38 ± 0.08	0.079 ± 0.02	0.060 ± 0.02
1000 ± 150	0.12 ± 0.02	0.94	0.75 ± 0.15	0.048 ± 0.01	0.045 ± 0.01

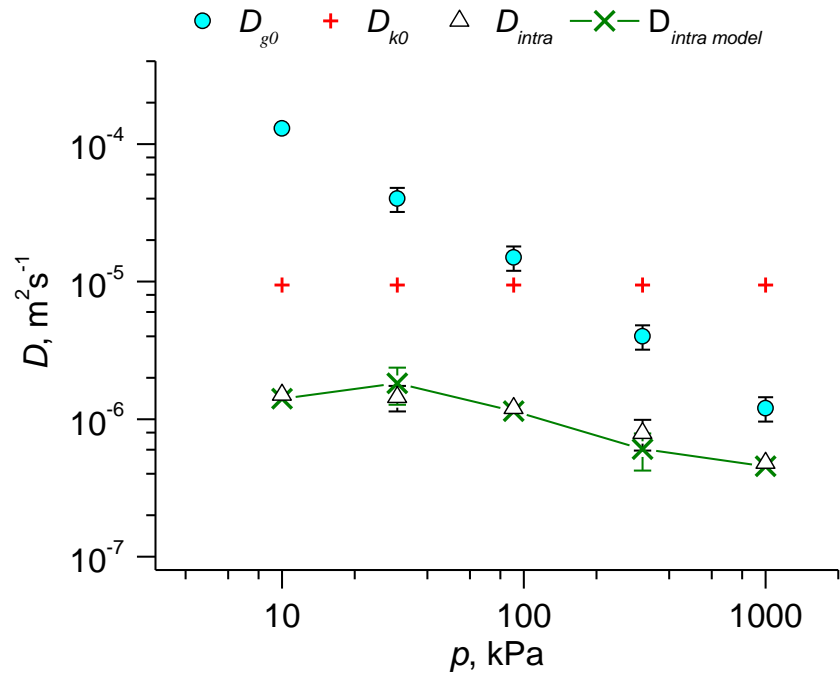


Figure S1. CO_2 self-diffusivity, D_{intra} , measured by ^{13}C PFG NMR inside the particles of the studied samaria aerogel catalyst at 297 K and the corresponding theoretical diffusivity, $D_{intra\ model}$, obtained by least-squares regression of the diffusion data reported in the figure to the modified Eq. 9 where $\eta_K = \eta_g \equiv \eta$. Also shown for comparison are the following self-diffusivities of CO_2 molecules at 297 K: self-diffusivity in the macroscopic gas volume surrounding the catalyst (D_{g0}), and the reference self-diffusivity in the Knudsen regime estimated by using Eq. 2 with $d = 75$ nm (D_{K0}). All diffusivities are presented as a function of the CO_2 equilibrium pressure in the gas volume surrounding the catalyst particles at 297 K.