Water permeation through graphene nanoslit by molecular dynamics simulation

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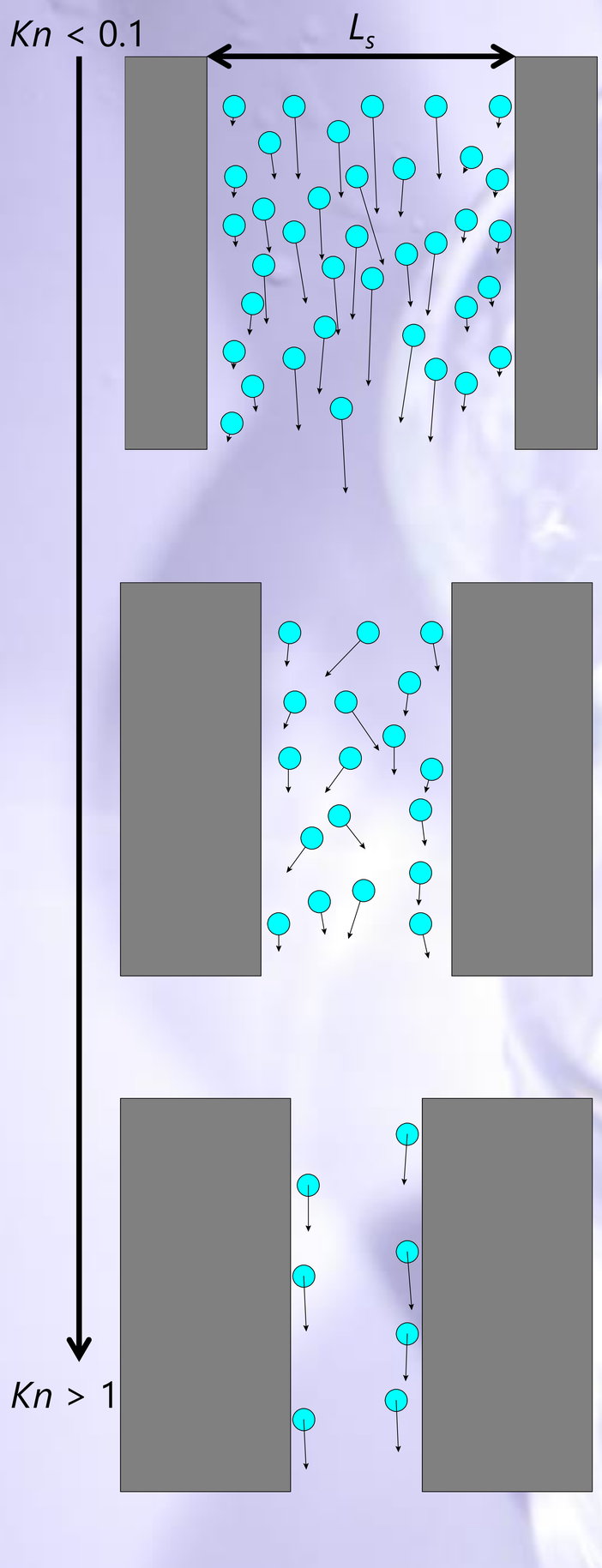
Objectives

The Knudsen number (*Kn*) is used to show the applicability of the laws of fluid dynamics. The applicability *Kn* has been experimentally established; however, the exact value at which the deviation occurs and the reason for it are not known.
We calculated the permeability of liquid water from MD simulations and compared the results with analytical models.

$$Kn = \frac{Molecular\ diameter}{Characteristic\ length}$$

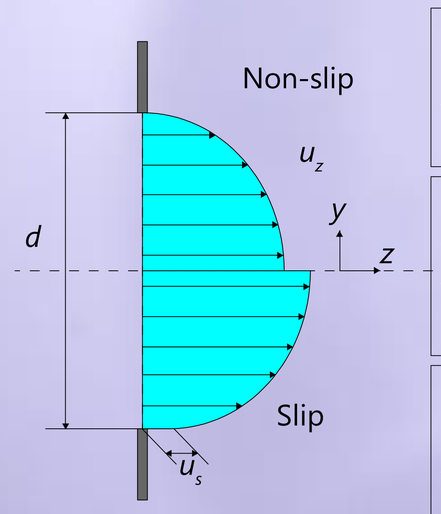


Continuum flow
The influence of the walls is negligible. Fluid dynamics is applicable.

Transition flow
Both continuum and free molecular flows occur. Fluid dynamics starts to fail.

Free molecular flow
The influence of the walls is relatively large. Fluid dynamics is not applicable

Permeability calculation



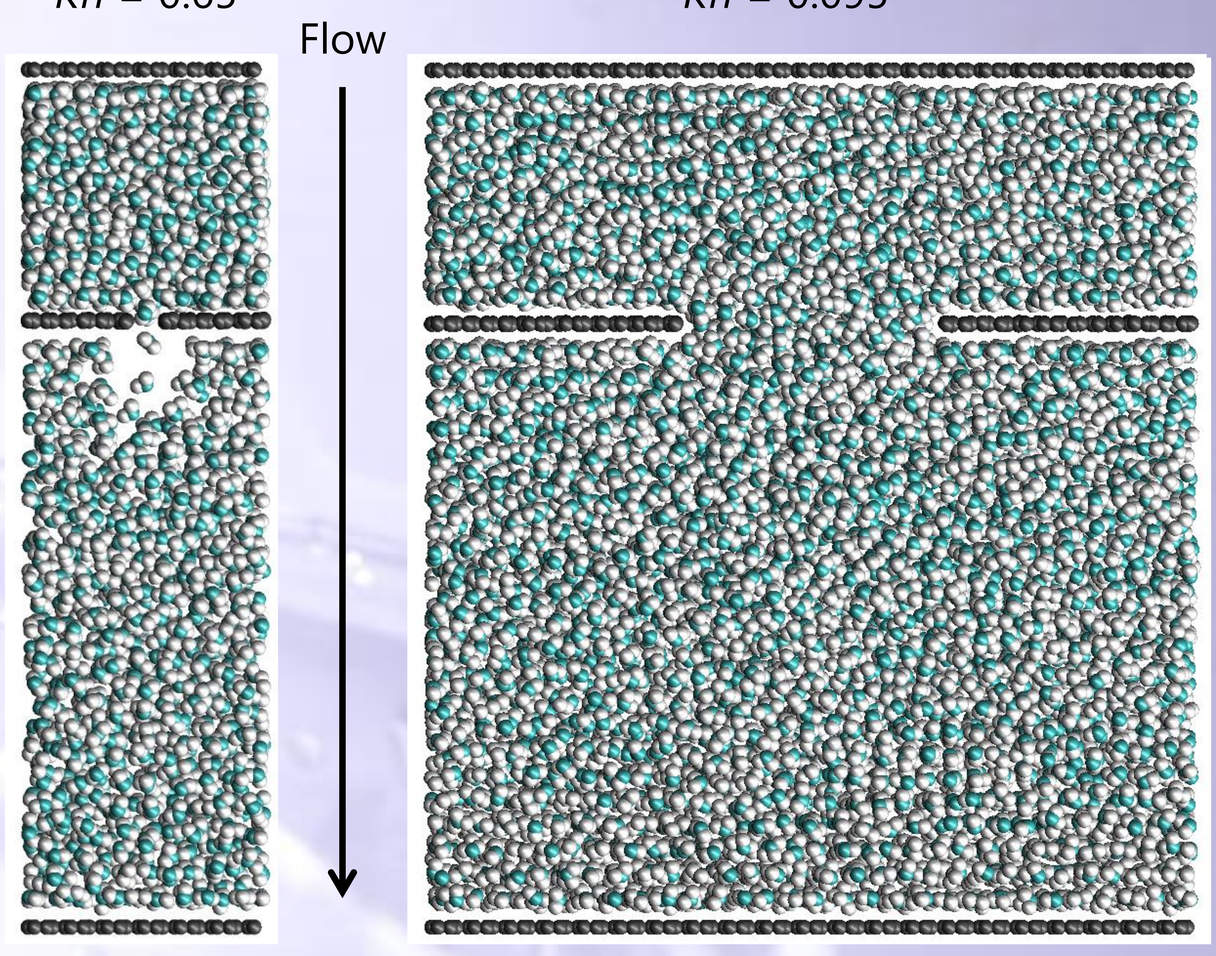
$$K_{MD} = \frac{Q}{\Delta P}$$

$$K_{non-slip} = \frac{\pi d^2}{32\mu}$$

$$K_{slip} = \frac{\pi d^2}{32\mu} + \alpha d \qquad \alpha = \frac{u_s}{\Delta P}$$

Q: Flow rate
ΔP: Pressure difference
d: Slit width
μ: Viscosity
u_s: Slip velocity

Results



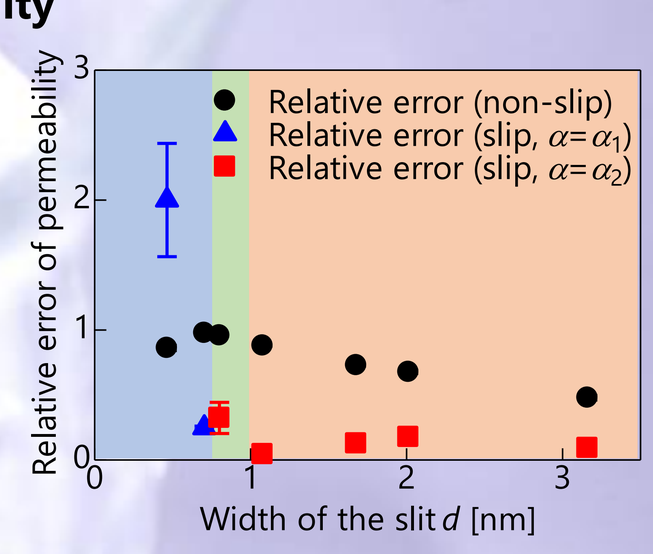
A non-continuum flow is observed for *Kn* = 0.65.

Relative error of permeability

***Kn* < 0.375**:
K_{MD} agrees well with K_{slip}.

***Kn* > 0.375**:
K_{slip} is not applicable.

※ α_1 and α_2 are the mean value of α at *Kn* > 0.375 and *Kn* < 0.375, respectively.



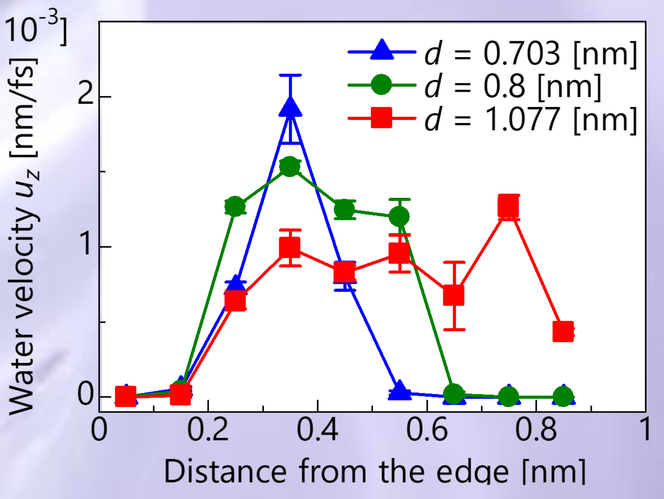
Fluid dynamics is not applicable at *Kn* > 0.375.

Velocity profile

***Kn* < 0.375**:
There are two peaks at 0.35 and 0.75 nm from the edge.

***Kn* = 0.375**:
There are no peaks.

***Kn* > 0.375**:
There is a peak at 0.35 nm from the edge.



Applicability changes with the number of high-velocity peaks.

Conclusion

At *Kn* > 0.375, fluid dynamics is not applicable. The flow changes from a continuum to free molecular flow when the permeation of the water molecules between the slits changes from multiple-layers to a single-layer.