Separation of light gases using soap-film membranes

Pablo Sanchez-Moreno Royer, Benoit Coasne, Elise Lorenceau

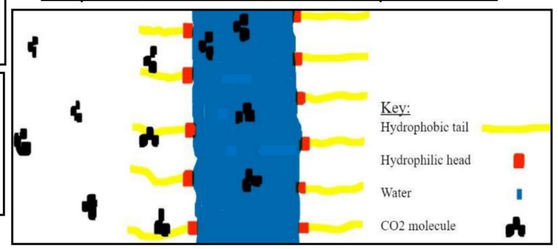
Laboratoire Interdisciplinaire de Physique, Saint-Martin D'Heres, France. Pablo.Sanchez-Moreno-Royer@etu.univ-grenoble-alpes.fr

Air filtration is a potential way to reduce greenhouse gas emissions

HOWEVER — Current air filters are:
-unrecyclable
-expensive
-inefficient

SO — Consider soap-film membranes. They are:
-recyclable
-cheap
-actually effective
-possibly very efficient

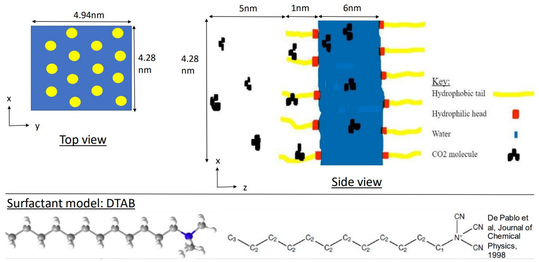
Soap-film membrane schematic representation



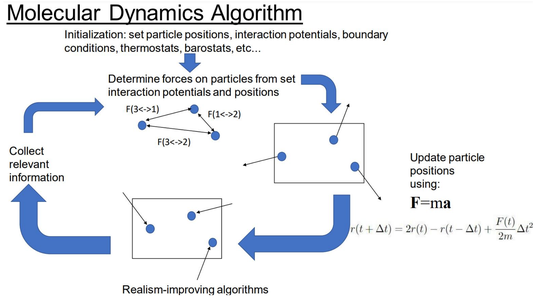
HOWEVER — 1) Gas permeation through them is not understood
2) Gas permeation cannot be observed *experimentally*

SO — GOAL: "Observe" gas permeation by using *simulations* of the membrane

Soap-film membrane model



Molecular Dynamics Algorithm



OBSERVING PERMEATION WAS TO BE DONE:

-visually

-by measuring the excess gas adsorption

INTERMEDIATE STEPS:

1) Build a model of a thin-liquid film with and without surfactant monolayers

2) Simulate the entire system in Grand Canonical Monte Carlo (GCMC) to insert and remove gas molecules, varying the pressure and the type of gas molecule

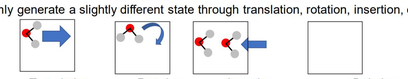
3) Determine the excess gas adsorption once the number of gas molecules is stable

4) Simulate the entire system in Molecular Dynamics (MD) for 2.5 nanoseconds and observe

Grand Canonical Monte Carlo Algorithm

1) Start in a stable state:

2) Randomly generate a slightly different state through translation, rotation, insertion, or deletion



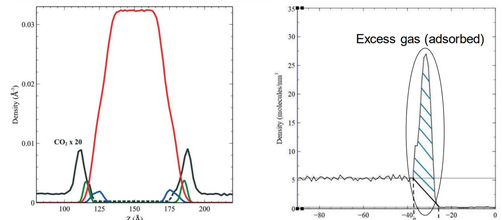
3) Calculate the transition probability:

$$P_T = e^{\beta(\Delta E - \mu \Delta N)}$$

4) Accept the new state with a probability acc(o->n)=min(1, exp(-β($\Delta\varepsilon$-$\mu\Delta$N)))

5) Update the state in case of acceptance (i.e.: stability), otherwise reject it

Excess Gas Adsorption



Density profile of different molecules in the soap-film membrane

Falciani et al, Molecular Systems Design and Engineering, 2020

Results

10000Pa

#/nm^2	CO2	N2	O2
S	1.2866	Unavailable*	Unavailable*
S0	0.2740	0.1198	0.1398

10000Pa

#/nm^2	CO2	N2	O2
S	9.3479	Unavailable*	1.1693
S0	11.219	1.0117	0.6304

100000Pa

#/nm^2	CO2	N2	O2
S	84.3444	1.1513	7.2180
S0	85.8037	3.6031	18.3390

Discussion

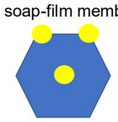
No permeation was ever observed

There were *too few gas molecules* for the excess gas adsorption's uncertainty to be at a satisfying value

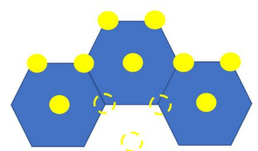
*There were *too few gas molecules* for the excess gas adsorption to be calculated

How to do it better

1) Build a model of a soap-film membrane in a hexagonal box



2) *If more gas molecules are needed*, tesselate the model in order to have more space:



3) Simulate the entire system in GCMC to insert and remove gas molecules, varying:

pressure - type of gas - number of types of gas

4) Determine the excess gas adsorption once the number of gas molecules is stable

5) Simulate the entire system in MD *until permeation is visible*