DD3R zeolite membranes in separation and catalytic processes

Modelling and application

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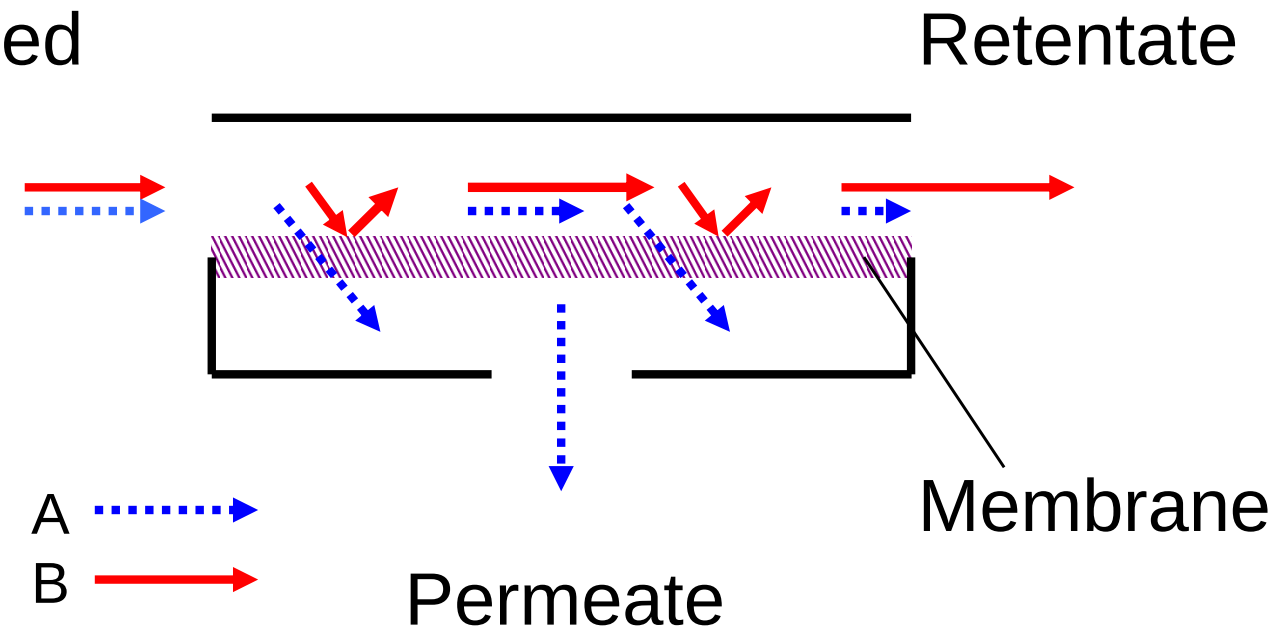
Algemene vergadering Bataafsch Genootschap

Motivation

- 15% of the world energy demand was required for separation processes to produce commodities (2009)*
  - A threefold increase of demand is expected in 2040
- Dutch (Petro)chemical industry energy consumption ~ 460 PJ (2004)**
  - ~200 PJ allocated to separation processes
- We need to evolve beyond the thermal age of separation processes*
  - Thermal = Energy loss
  - Membranes can lead the way

*W.J. Koros, Euromembrane 2009
**Innovation roadmap Scheidingstechnology, 2004

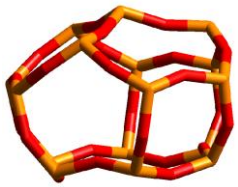
Membrane technology



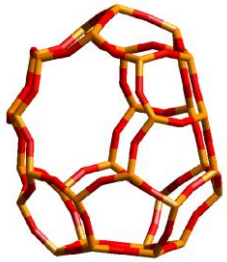
Simple, continuous operation, **energy-efficient**

Membrane material is key: selectivity, flux, stability, cost

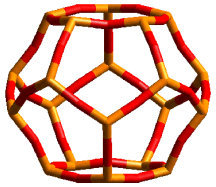
Zeolite DD3R



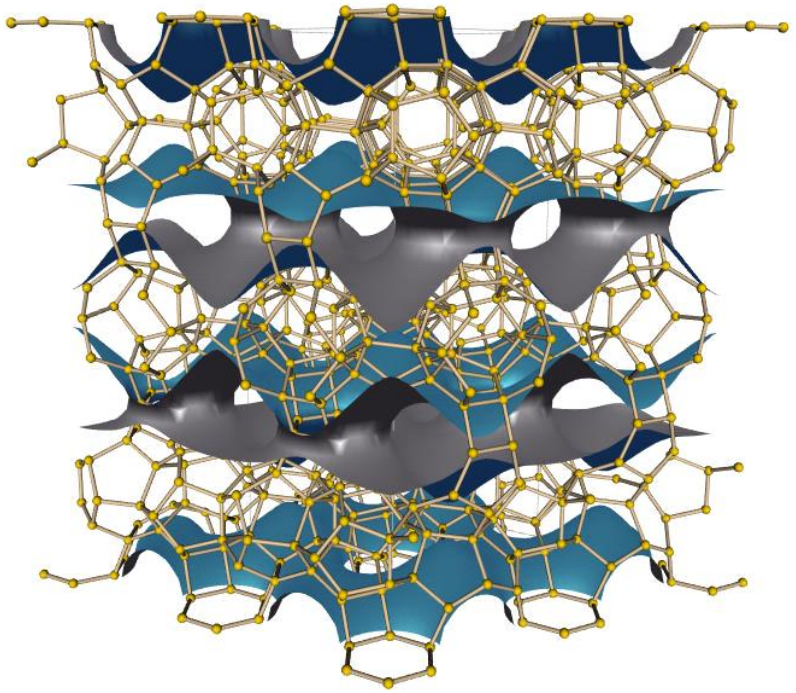
$[4^3 5^6 6^1]$ cavity
inaccessible



$[4^3 5^{12} 6^1 8^3]$ cavity
accessible

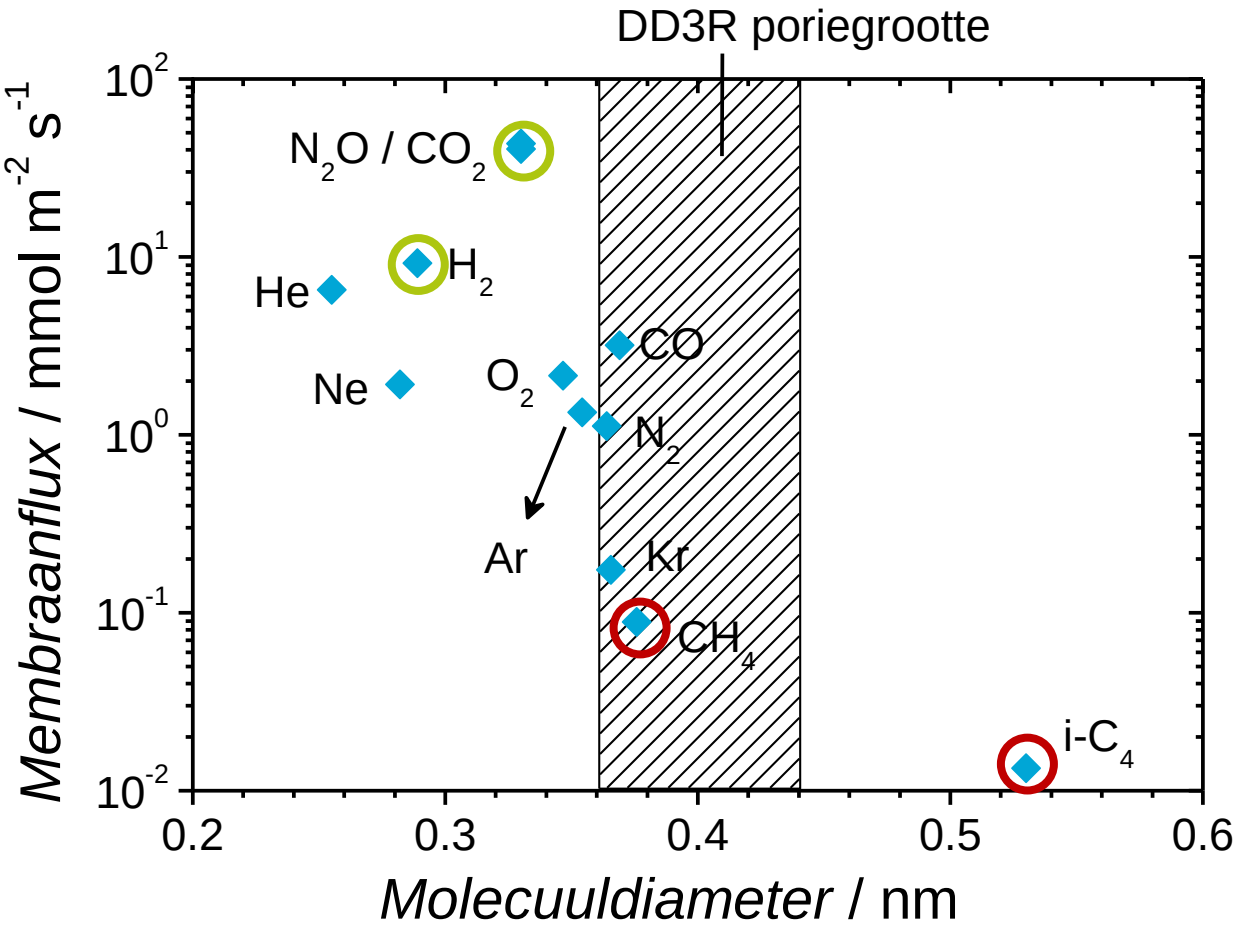


$[5^{12}]$ cavity
inaccessible



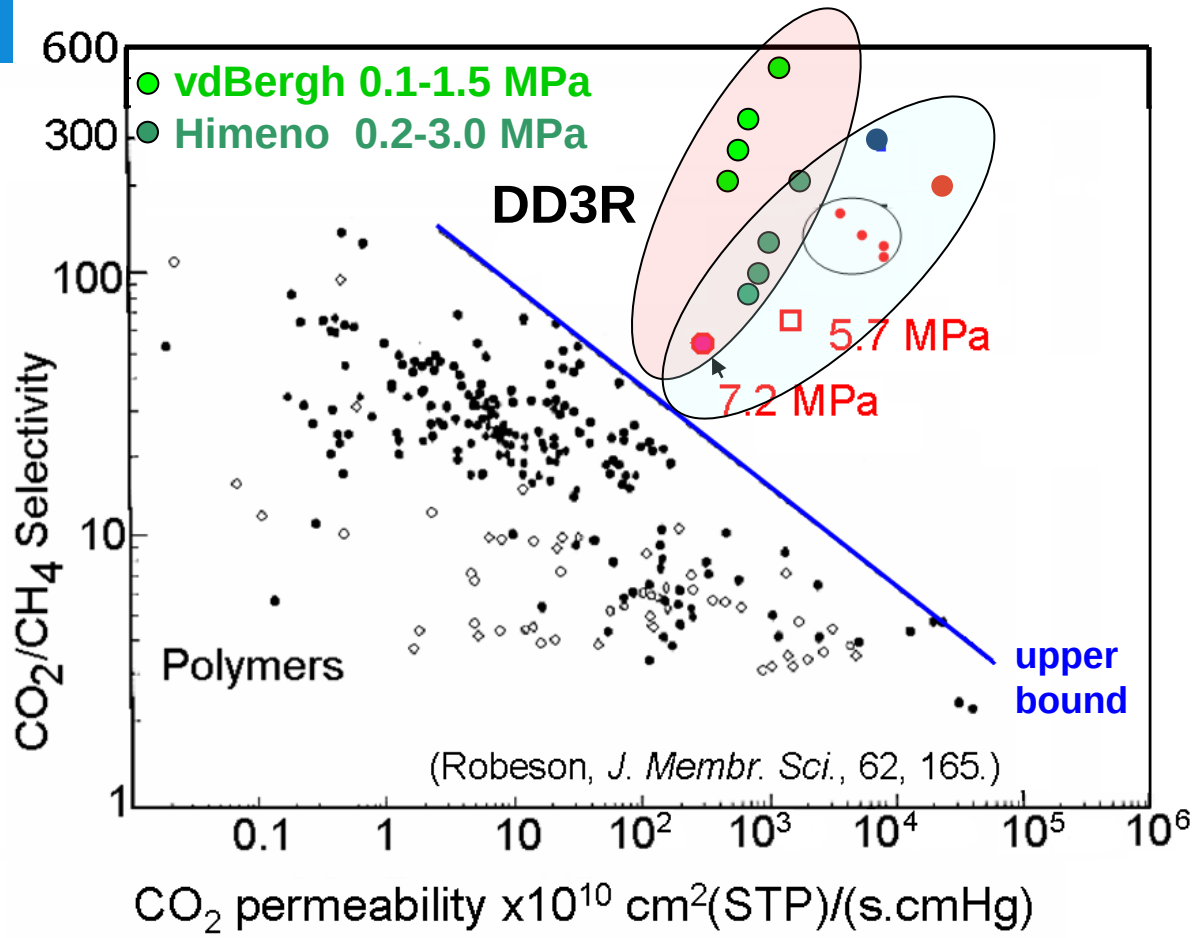
- Crystalline aluminosilicates
- Very high thermal and chemical stability
- Well-defined pore size of molecular dimensions

Molecular sieving



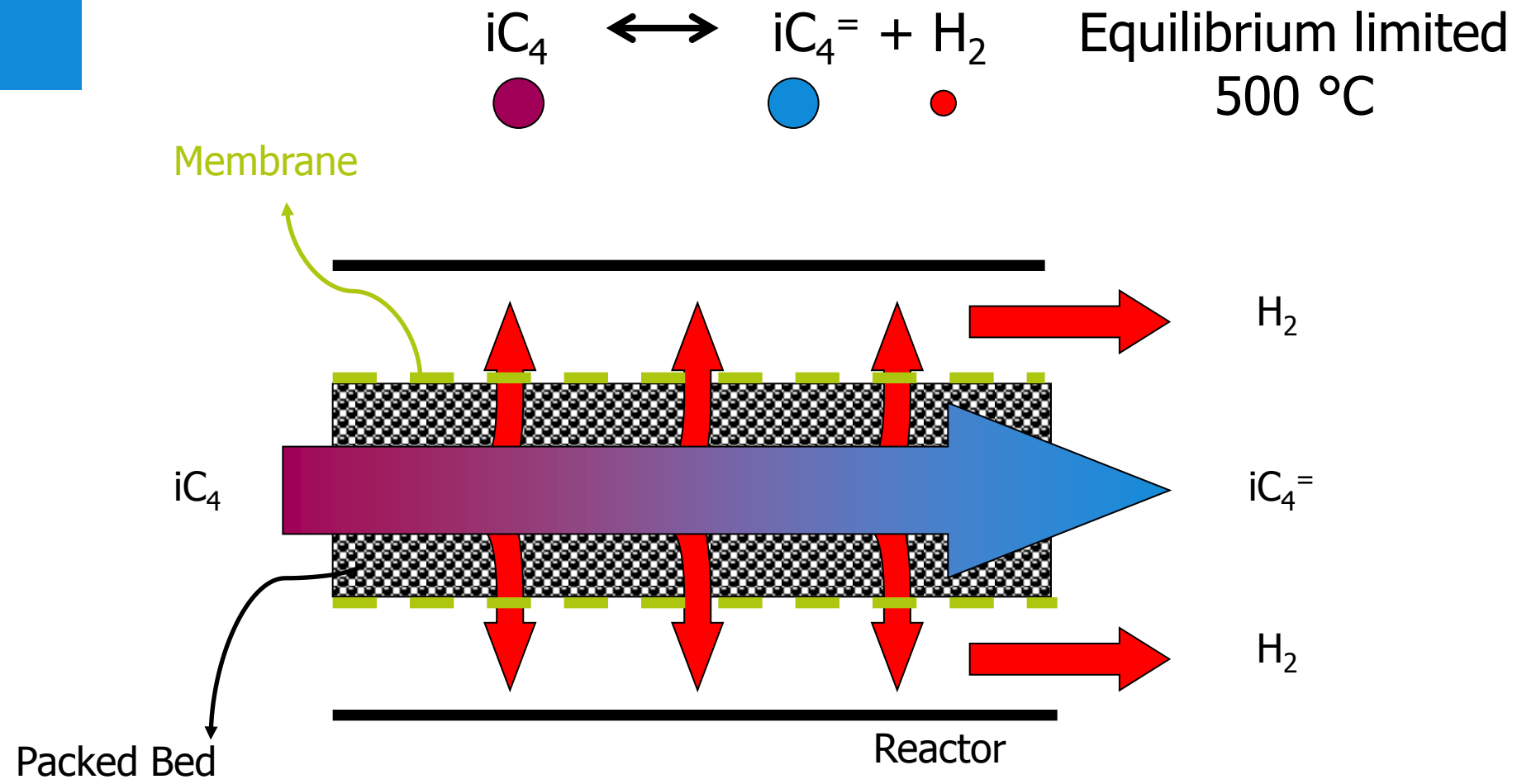
Promising separations: **CO_2/CH_4** and **H_2/hydrocarbons**

Natural gas purification
Robeson plot – CO_2/CH_4 @25 °C

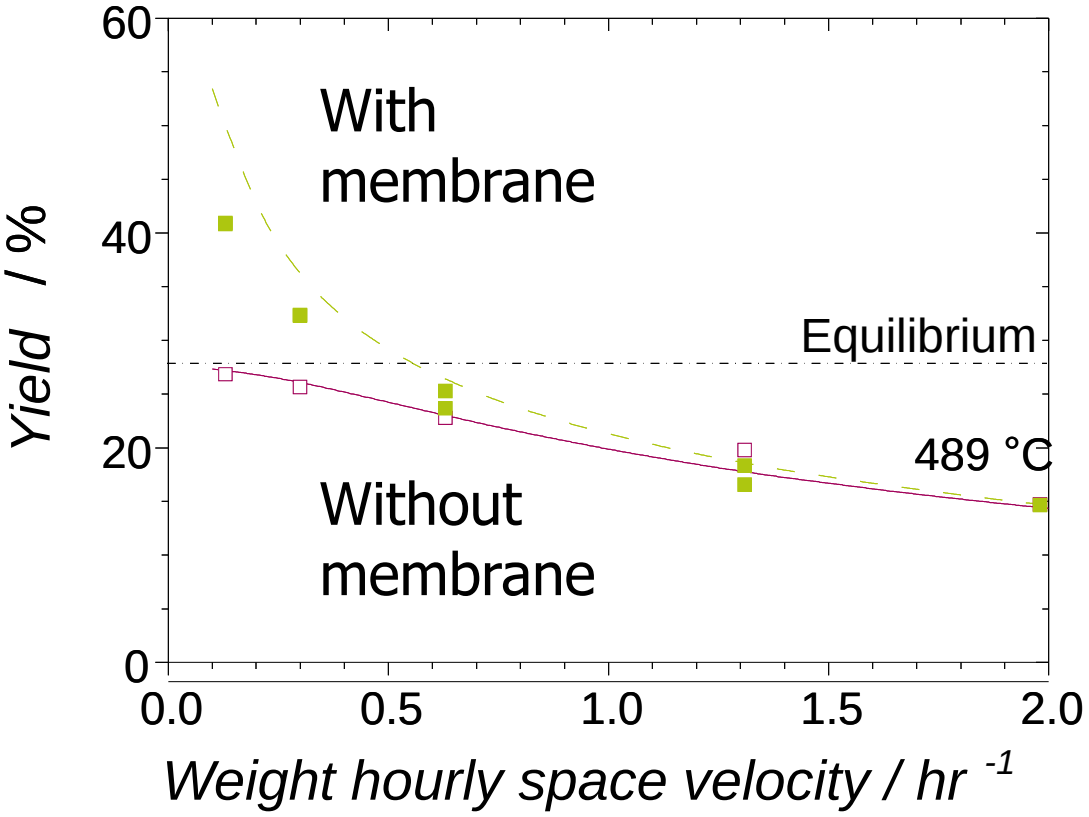


Zeolite membranes break upper bound for polymer membranes

Membrane reactor concept



Membrane reactor results

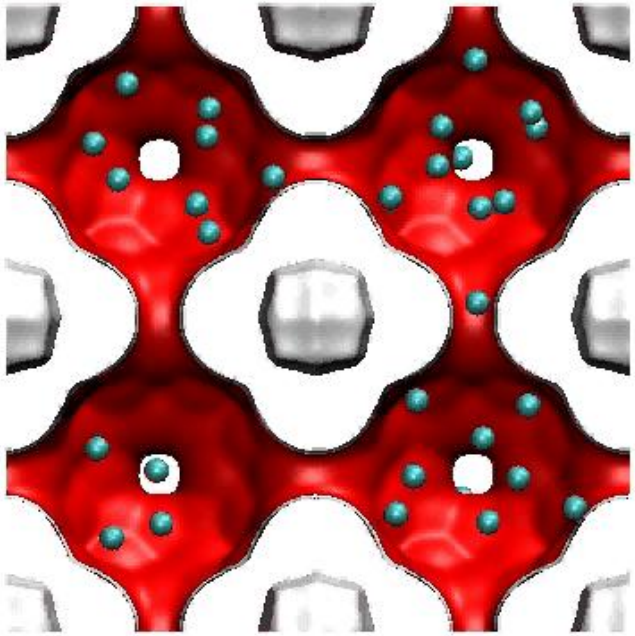


Membrane increases yield

Stable operation at high temperature!

Modelling mass transport

Nanoscale (molecules)



Molecular dynamics

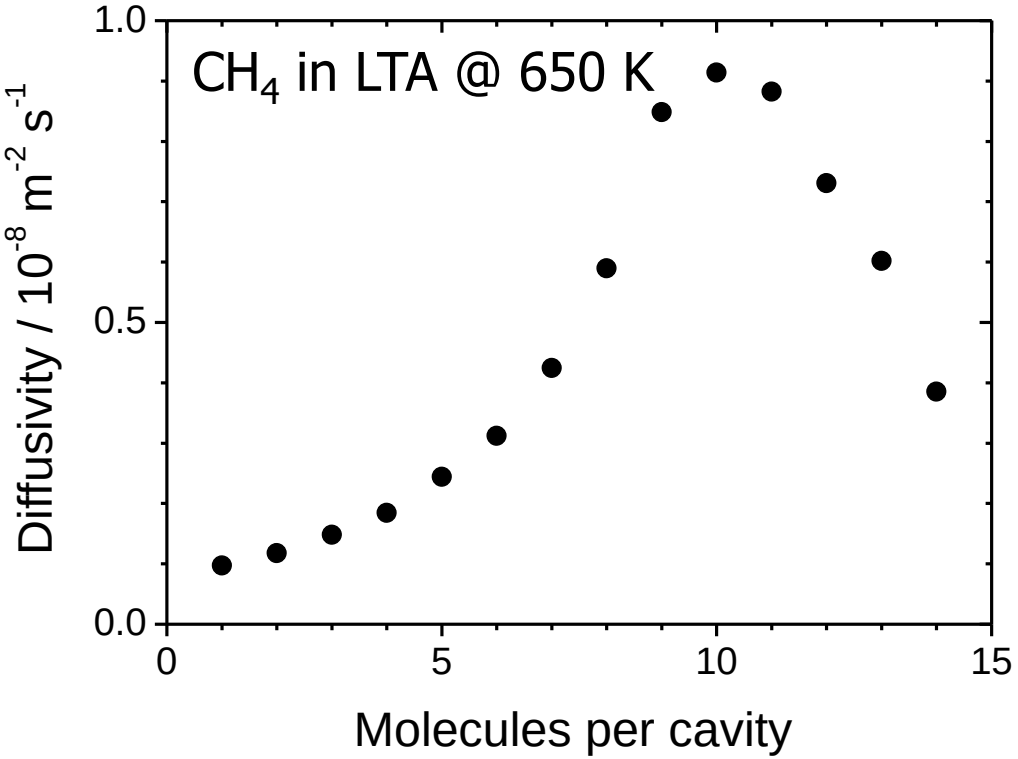
Model

Macro-scale (Design)

http://www.science.uva.nl/research/cr/animateMD/

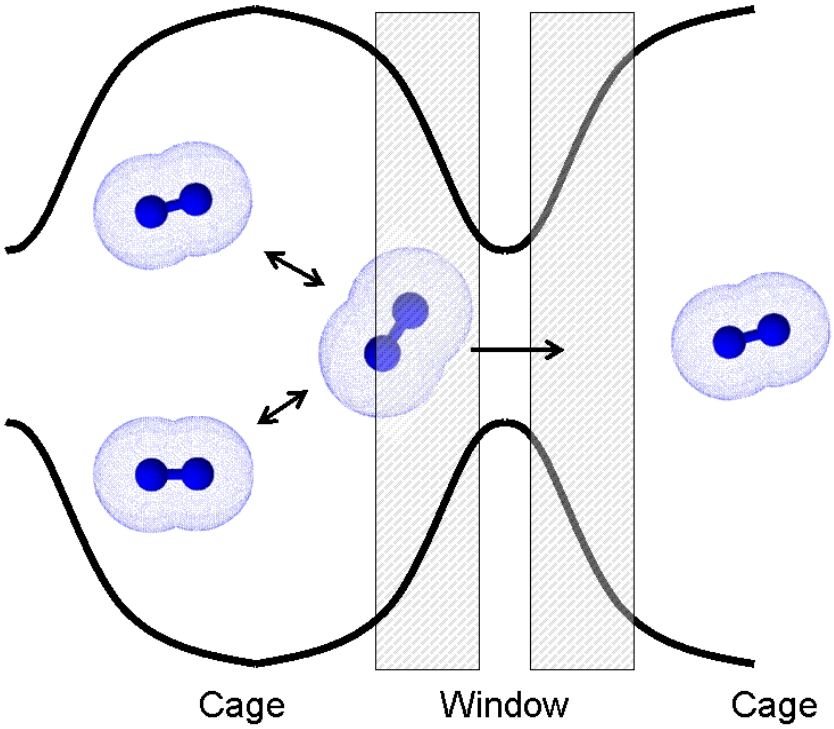
Diffusivity (D) concentration dependent

$$Flux = f(D, c, ..)$$



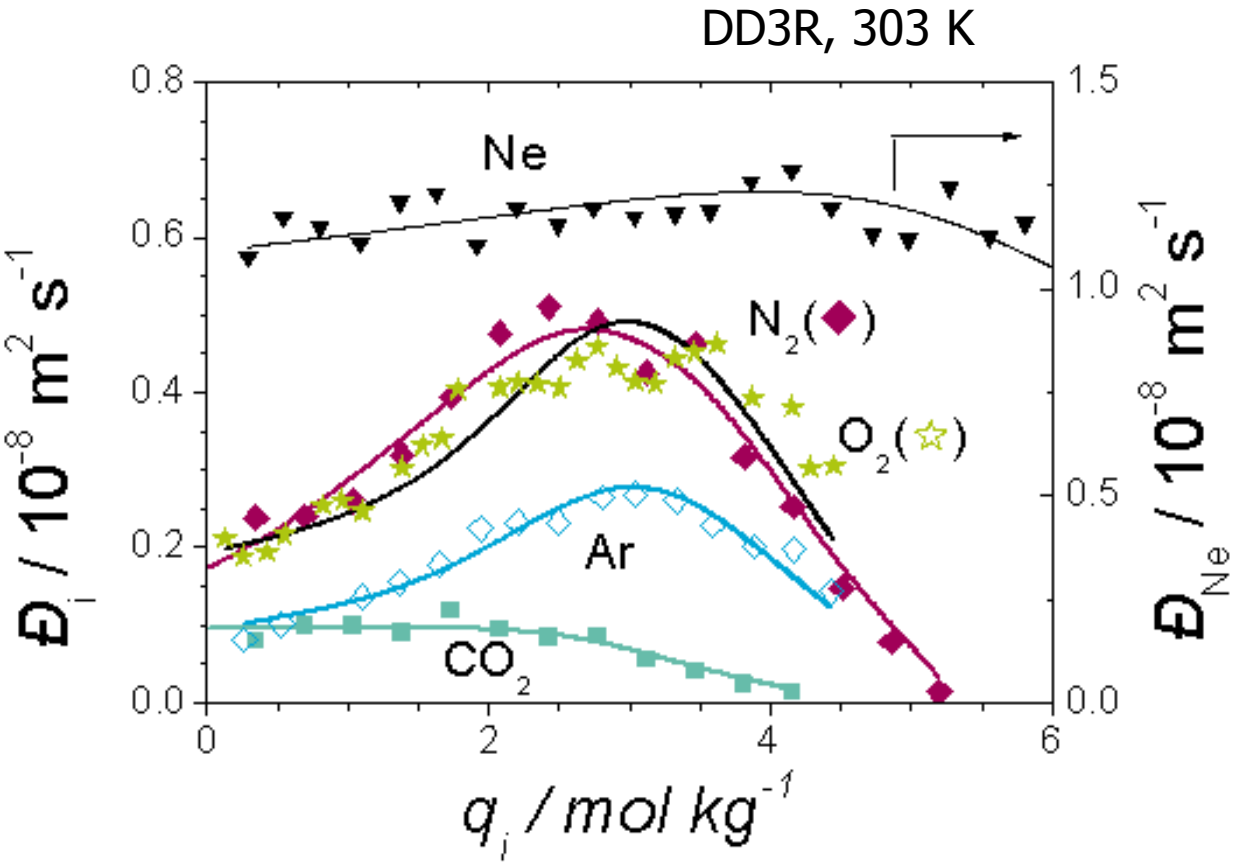
D. Dubbeldam *et al.*, *The Journal of Chemical Physics*, 122, **2005**, 224712.

New model: Relevant Site Model

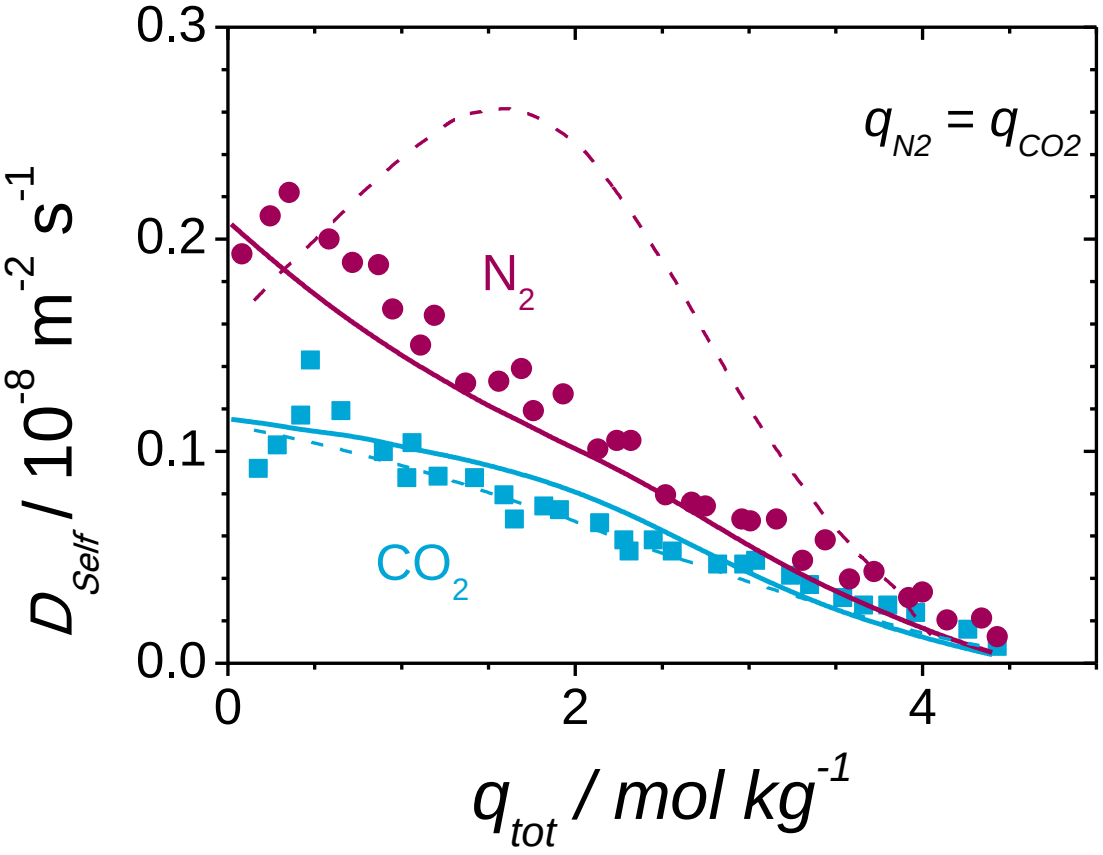


- Concentration inside a zeolite is segregated
- A new model is derived that accounts for this

Excellent description of single component data



Mixture predictions: CO_2/N_2 in DDR



Data: R. Krishna and J. M. van Baten, *Chemical Physics Letters*, 446, **2007**, 344.

Results summary

- DD3R zeolite membranes:
  - Stable, high performance membranes
  - **Natural gas purification**
  - **Membrane reactor** -> dehydrogenation reactions
- Zeolite membranes: from potential to applications

- New model to describe diffusion in zeolites
  - Provides **new insights** in diffusion in zeolites
  - Important step forward in modelling mass transport in zeolite membranes

DD3R zeolietmembranen in scheiding- en katalytische toepassingen

Modellering en toepassing

Johan van den Bergh, 21 September 2010