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Advanced Membrane Reactors: Modelling the use of CO_2 versus H_2 selective membranes

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Introduction

Power production with CO_2 capture from fossil fuels can be done with membrane reactors using either CO_2 or H_2 selective membranes. In the GCEP programme both types are under investigation. Membrane reactors can be both membrane reformers as well as water gas shift membrane reactors.

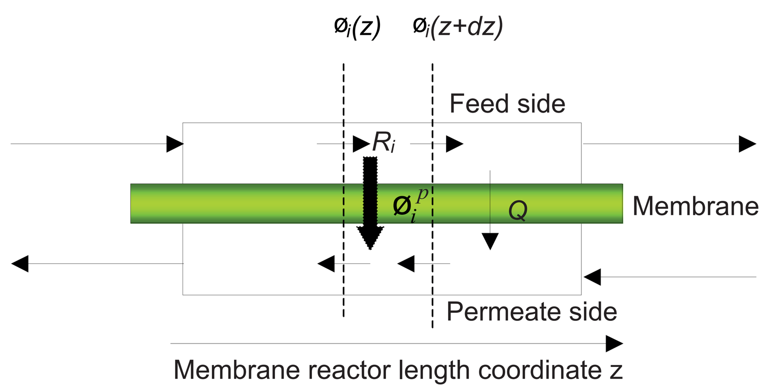
Working principle

A hydrocarbon mixture is being converted to H_2 and CO_2, while (depending on the type of membrane used) either H_2 or CO_2 are separated simultaneous to the reaction. This increases conversion and allows for more advantageous temperatures of reaction. The CO_2 is available for storage, H_2 can be used for power production.

Membrane reformer	$CH_4 + 2H_2O \rightarrow 4\ H_2 + CO_2$
Water gas shift membrane reactor	$CO + H_2O \rightarrow H_2 + CO_2$

Modelling

The comparison is done on a reactor level using a 1-dimensional reactor model. The model consists of partial differential equations describing mass balances, heat balances, chemical reaction kinetics, permeation and heat transfer.



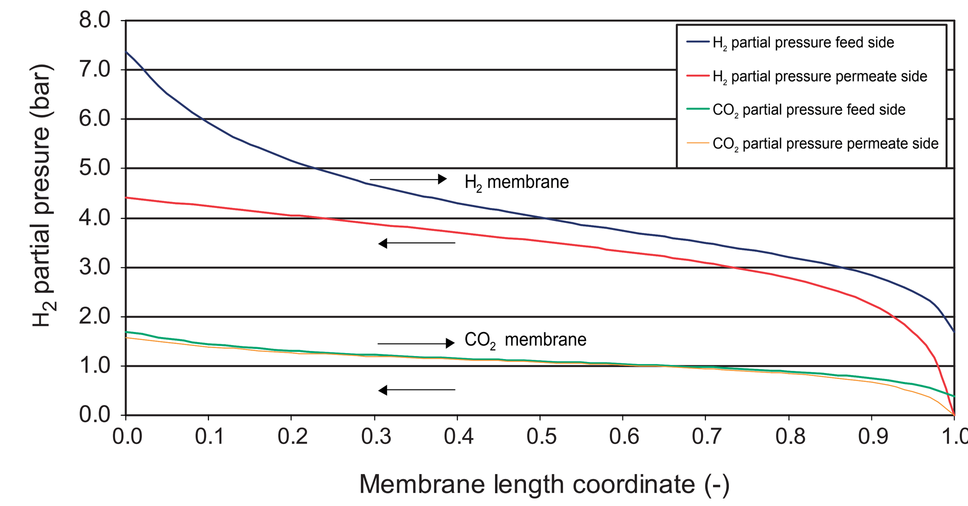
$$\phi_i^p(z) = Q_i\,(T) * A_{mem} * \left[p_i^{feed\ side}(z) - p_i^{permeate\ side}(z)\right]$$

Membrane reformer data
Feed: CH_4, 44000 kg/h pre-reformed at 600°C (~600 MW_{th}), 40 bar, S/C = 3, excess catalyst
Sweep: steam 5 bar, 600°C, Sweep flow/Feed flow = 0.11 (mole/mole)
Membrane: selectivity 100%, A_{mem} = 5000 m^2, permeance H_2 and CO_2 Q= 2*10^{-6} mol/m^2.s.Pa

Water gas shift membrane reactor data
Feed: product gas from Texaco coal gasifier (~600 MW_{th}) cooled to 300°C, 42.2 bar, S/C just enough to complete water gas shift, excess catalyst
Sweep: steam 17 bar, 300°C
Membrane: selectivity 100%, A_{mem} = 50 000 m^2, permeance H_2 and CO_2, Q= 1*10^{-6} mol/m^2.s.Pa

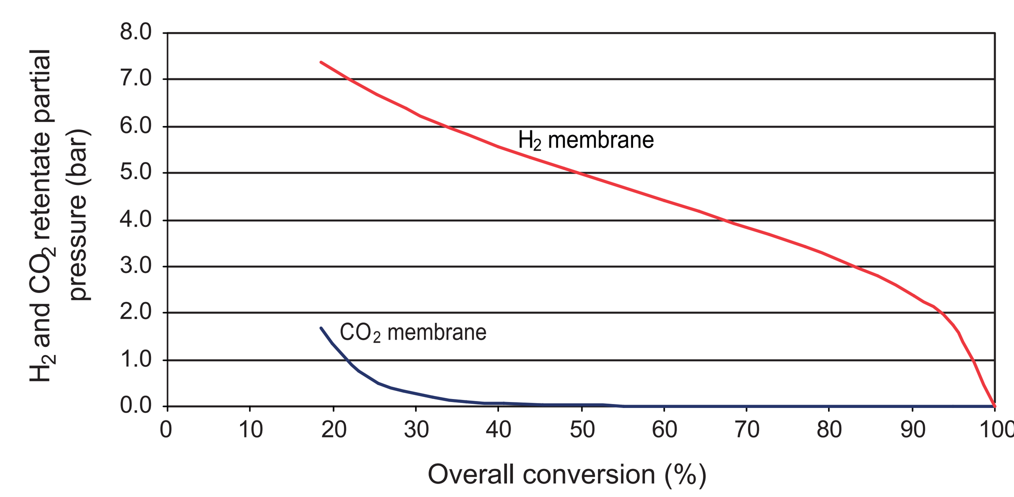
Partial pressure profile: membrane reformer cases

The driving force for H_2 permeation is high for CO_2 low.



Conversions membrane reformer

CO_2 has to be removed to extremely high levels for acceptable conversions.

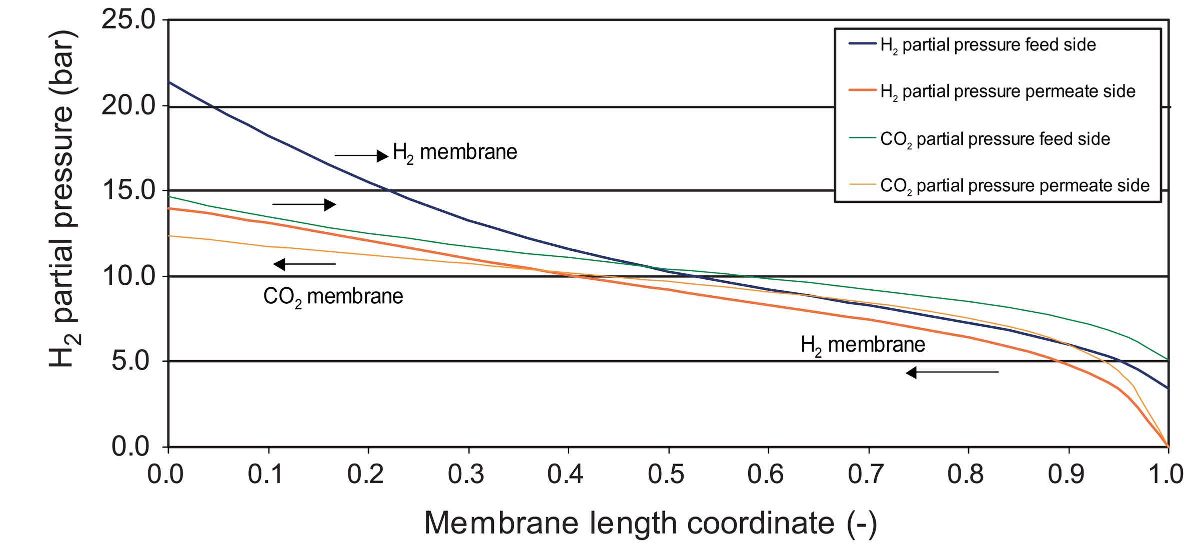


Conclusions

<u>Membrane reformer</u>: CO_2 selective membranes show a too low conversion and are therefore not suitable, as opposed to H_2 selective membranes.
<u>Water gas shift membrane reactor</u>: CO_2 selective membranes give conversions comparable to H_2 separating membrane and offer therefore a viable alternative.

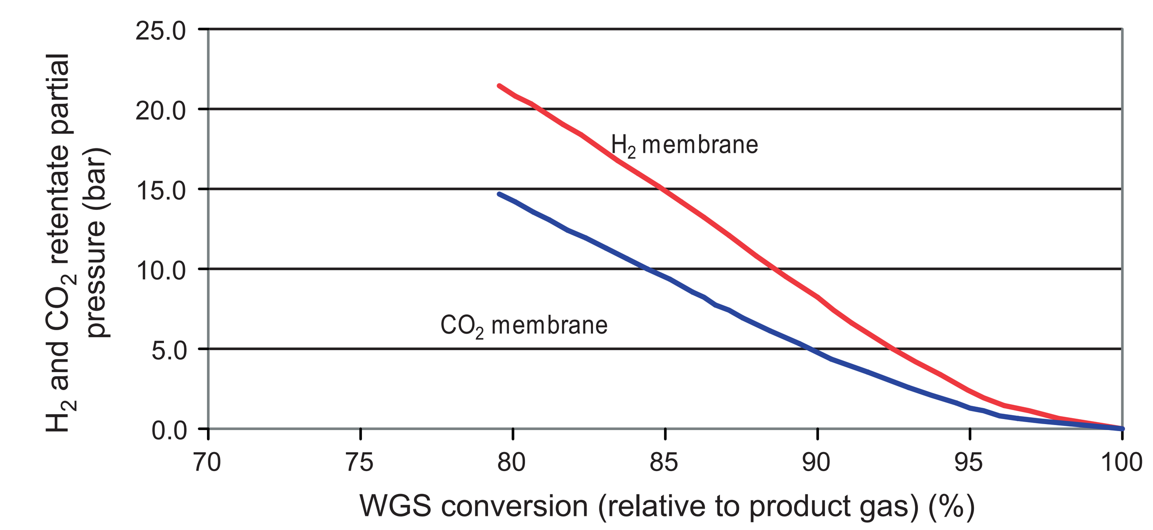
Partial pressure profiles: water gas shift membrane reactor cases

The driving forces for H_2 and CO_2 permeation are similar.



Conversions water gas shift membrane reactor

CO_2 and H_2 removal are similar.



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