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Chemical & Biological Engineering

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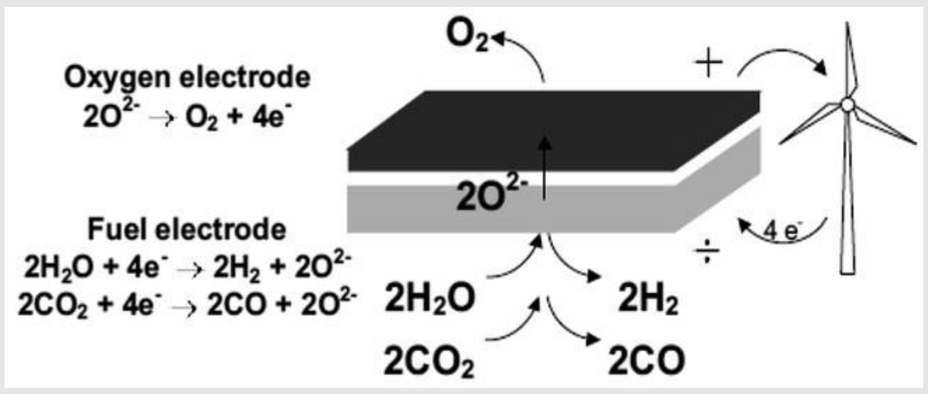
CO_2/H_2O Co-electrolysis in solid oxide electrolysis cells: A modelling approach

1. Background

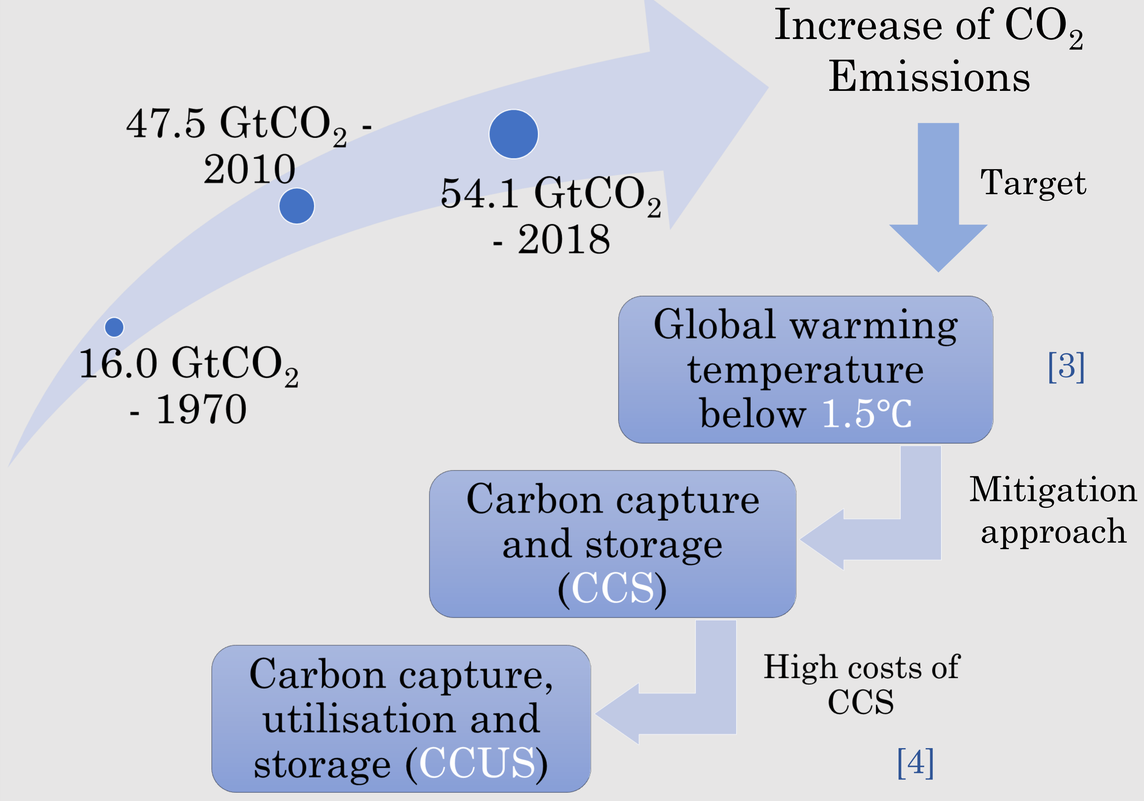
- Solid oxide electrolysis cells (SOECs) are devices that use renewable electricity to convert CO_2 and H_2O into CO and H_2 via co-electrolysis. [1]



[2]

- SOECs Operate at high temperatures (above 700°C) which reduce their need in electricity.

2. A broader context

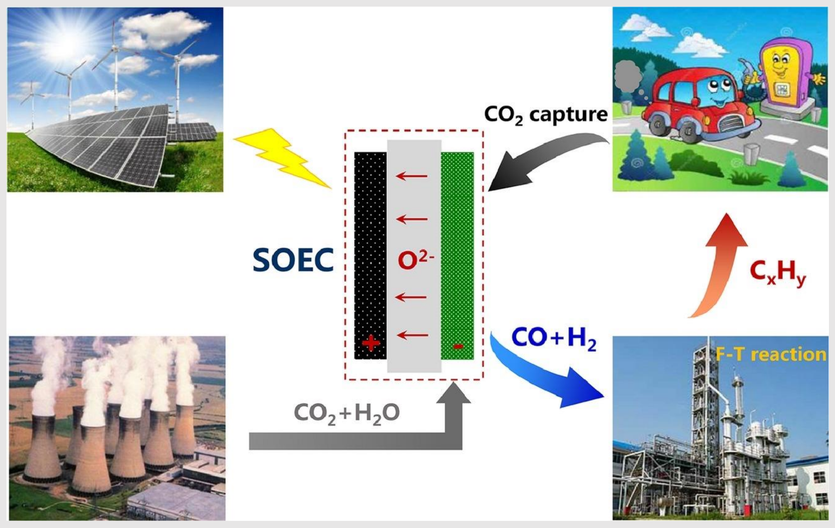


3. The problem

There are 3 main challenges hindering SOEC commercial deployments: [5]

- Effective activation of CO_2 molecule
- Degradation occurring at the electrodes
- Integration of SOEC device to clean electricity grid

The big picture



[6]

- Syngas ($CO+H_2$) produced from SOEC can be processed into liquid fuels via Fischer-Tropsch (F-T) process.

4. Methods

Modelling and simulation approaches:

- Further understanding of reaction mechanisms;
- Design and optimization of processes;
- Less use of reagents thus lower cost.

Modelling & Simulation → Model validation → Process analysis

Comparison of model and experiment results

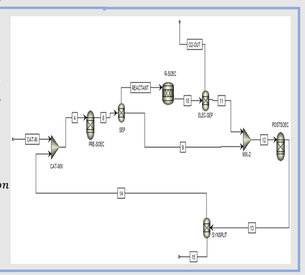
- Model development

$$\dot{N}_O = \frac{I}{n \times F} = \frac{A_{tot} \times j}{n \times F}$$

$$\dot{N}_O = \xi_{CO_2} + \xi_{H_2O}$$

$$U_{SOEC} = U_N + U_{act} + U_{ohm} + U_{con}$$

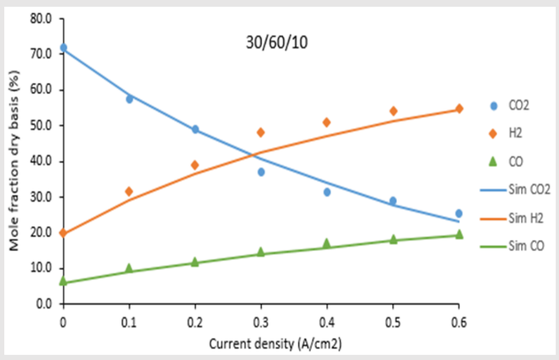
- Process design and integration



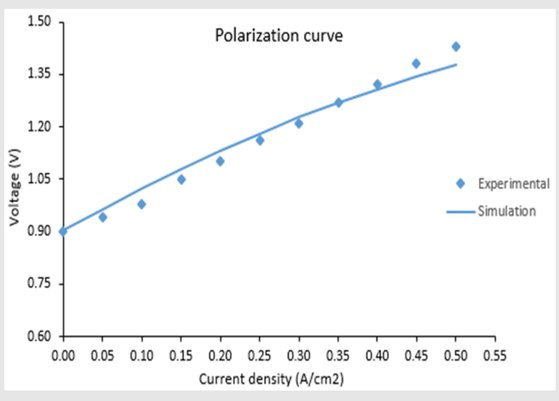
- Contribution of CO_2
- Degradation mechanism
- Performance analysis (energy, conversion etc.)

5. Results

Model validation



- Outlet gas: Max error is 11.5% at 0.3 A/cm²



- i-V curve: Max error is 4.0% at 0.3 A/cm²

6. Conclusion

- In addition to CCS, it is pertinent to evaluate the economic value of CO_2 through utilisation.
- One potential solution is to produce liquid fuel from CO_2 and H_2O using SOEC.
- So far, a steady-state SOEC model has been developed and simulated in Aspen Plus®. The model was also validated for the outlet composition and polarisation (i-V) curve with the highest error of 11.5% and 4.0%, respectively.
- Future work include SOEC process analysis and integration with electrical grid.

References

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[2] Hansen, J. (2015), Solid oxide electrolysis – a key en abling technology for sustainable energy scenarios, *Faraday Discussions*, Vol. 182, p.9-48.

[3] IPCC (2018), Special report - Global warming of 1.5 °C, [online] Intergovernmental Panel on Climate Change. Available from <https://www.ipcc.ch/sr15/> [19 June 2019]

[4] Rodrigues, C., Dinis, M. and Lemos de Sousa, M. (2015), Review of european energy policies regarding the recent "carbon capture, utilization and storage" technologies scenario and the role of coal seams, *Environmental Earth Sciences,* Vol. 74 (3), p.2553-2561

[5] Zhang, Y., Wang, J., Yu, B., Zhang, W., Chen, J., Qiao, J., Zhang, J. (2017), A review of high temperature co-electrolysis of H_2O and CO_2 to produce sustainable fuels using solid oxide electrolysis cells (SOECs): advanced materials and technology, *Chem. Soc. Rev.*, Vol. 46, p.1427-146

[6] Zhang, X., Song, Y., Wang, G. and Bao, X. (2017), Co-electrolysis of H_2O and CO_2 in high-temperature solid oxide electrolysis cells: Recent advance in cathodes, *Journal Of Energy Chemistry* Vol. 26 (5), p. 839-853