Supporting information: Overcoming the Energy-Water Nexus in Dry Regions - Water-Positive Production of Green Hydrogen Carriers and Base Chemicals: the DryHy project - Technical Aspects

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1 Thermodynamic safe region

The methodology for the calculation of the thermodynamic safe region in the main article is presented here (c.f. Figure 4 in the main article). A simplified block diagram of the solid oxide electrolysis cell (SOEC) is given in Figure 1.

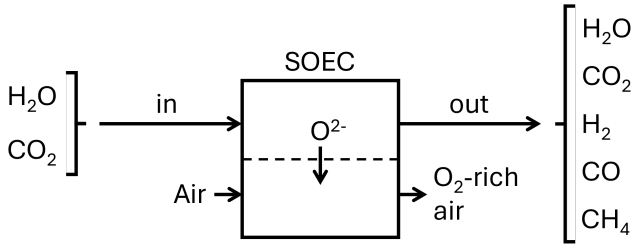

Fig. 1 Simplified block diagram of a solid-oxide electrolysis cell.

For the operation of a solid-oxide electrolysis cell (SOEC) in co-electrolysis mode the following definition of utilization was selected: number of oxygen atoms removed through the membrane divided by the number of H_2O and CO_2 molecules at the inlet. Therefore a gas mixture of only water and CO_2 corresponds to a utilization of 0 and a (theoretical) mixture of only H_2 and CO corresponds to a utilisation of 1.

The chemical equilibrium for the gas phase at a given temperature and pressure is calculated by minimizing the total Gibbs energy as described by Gordon et al.[1]. The activity of carbon, α, is then calculated by the gas phase composition based on the Boudouard reaction as shown in equation 1.

$$\alpha = \exp\left(\frac{2g_{CO} - (g_{CO_2} + g_C)}{R_m \cdot T}\right) \cdot \frac{x_{CO}^2}{x_{CO_2}} \cdot \frac{p}{p_0} \quad (1)$$

Where g_i are the molar Gibbs free energies, x_i the molar fractions in the gas phase and T and p temperature and pressure respectively. p_0 is the reference pressure (here 1 bar).

When α has a value of 1 the gas phase is in thermodynamic equilibrium with solid carbon (graphite). The code for calculating the gas phase equilibrium and carbon activity is implemented in MATLAB. Thermodynamic gas properties are sourced from Daubert et al.[2] and thermodynamic data for graphite from the NIST-JANAF Thermochemical Tables[3].

Notes and references

1 S. Gordon and B. J. McBride, *Computer Program for Calculation of Complex Chemical Equilibrium Compositions and Applications. Part 1: Analysis*, NASA Lewis Research Center NASA Reference Publication NASA-RP-1311, 1994.

2 T. E. Daubert and R. P. Danner, *Physical and Thermodynamic Properties of Pure Chemicals: Data Compilation*, Hemisphere Publishing Corporation, New York, NY, 1989.

3 J. M. W. Chase, *NIST-JANAF Thermochemical Tables*, National Institute of Standards and Technology Technical Report J. Phys. Chem. Ref. Data, Monograph No. 9, American Chemical Society; American Institute of Physics for the National Institute of Standards and Technology, Gaithersburg, MD, 1998.

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