Liquid water scavenging of PEMFC contaminants

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The proton exchange membrane fuel cell (PEMFC), a cleaner alternative power generating device, still requires durability improvements to replace the incumbent internal combustion engine in automotive applications. Degradation is partly due to contaminant ingress because the system is open to the ambient atmosphere (1). However, the scavenging effect of the product liquid water on the numerous (2) and in some cases soluble contaminant species (Fig. 1) has not been studied.

The relevant time scales indicate that the liquid water accumulation in the gas diffusion electrode (3) is much slower than other time scales that include diffusion in the gas or liquid phase and contaminant absorption in the liquid phase (interface transport). Thus the liquid water phase is always saturated with the contaminant (equilibrium between gas and liquid phases). Under this condition, a contaminant mass balance leads to the following contaminant concentration expression assuming the ideal gas law, an isobar, isothermal and saturated gas stream, Henry’s law, the absence of water crossover, a constant volumetric gas flow rate, a uniform current distribution and the absence of a contaminant reaction:

\[ \frac{c(x)}{c(0)} = \frac{1}{1 + W_{i} \cdot x} \]  

[1]

where \( c \) represents the contaminant concentration, \( x \) the dimensionless flow field channel length and \( W_{i} \) a parameter defined by:

\[ W_{i} = nAc_{k}R_{O_{2}}/r \]  

[2]

where \( n \) represents the number of electrons exchanged for product water, \( A \) a solubility constant (Henry’s law), \( c_{k} \) the dry inlet gas concentration, \( R_{O_{2}} \) the fraction of oxygen in the dry inlet gas stream and \( r \) the reactant stoichiometry. The average contaminant concentration is calculated by integrating Eq. 1:

\[ \bar{c} / c(0) = \ln[1 + W_{i}] / W_{i} \]  

[3]

where \( \bar{c} \) represents the average contaminant concentration. For \( W_{i} \) equal to 2.51, the average dimensionless contaminant concentration is equal to 0.5. Fig. 2 indicates that the scavenging effect widely varies with the contaminant and is very significant especially for the relevant ethylene glycol species (an automotive coolant). Extension of this model to a generic single ionization reaction (contaminant species dissociation) demonstrates the importance of this process for low contaminant concentrations. Sulfur dioxide is a model air pollutant. The extended model shows a significant SO\(_{2}\) scavenging effect by dissociation below 0.2 ppm (4):

\[ \text{SO}_{2} + \text{H}_{2}\text{O} \rightarrow \text{H}_{2}\text{SO}_{3} \]  

[4]

\[ \text{H}_{2}\text{SO}_{3} + \text{H}_{2}\text{O} \rightarrow \text{H}_{3}\text{O}^{+} + \text{HSO}_{3}^{-} \]  

[5]

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REFERENCES


Fig. 1. Contaminant X transport pathways. The gas phase contamination path follows the flow field channel and an empty gas diffusion electrode pore to the ionomer and the catalyst. Along the same path the contaminant X dissolves into liquid water drops located in the flow field channel and a partially filled gas diffusion electrode pore decreasing the average contaminant concentration.

Fig. 2. Dimensionless contaminant concentration in the liquid water (Eq. 1) as a function of the dimensionless flow field channel length \( x \) and parameter \( W_{i} \) (Eq. 2).