SIMULATION OF DEGRADATION OF IrO_2 BY µ-KINETIC MODELLING AS ANODE CATALYST IN AEM-WATER ELECTROLYZERS

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ABSTRACT

The growing effects of global warming attributed to the increase of CO_2 and other greenhouse gases in the atmosphere originating from human industry enhances the motivation to find suitable replacements. Hydrogen has long been an attractive energy replacement for fossil fuels, and catalytic splitting of water through water electrolysis provides a way of producing hydrogen without CO_2. Anion-exchange membrane water electrolysers (AEM-WEs) aim to combine the advantages of established water electrolysers by combining alkaline operation with anionic-specific membranes. Still, AEM-WEs are relatively new but have the potential to produce energy- and cost-efficient hydrogen using more abundant catalyst materials. One of the problems with AEM-WEs is the stability of the catalyst.

A mechanism proposed by Kasian *et al.* [1] which describes both iridium dissolution and oxygen evolution on IrO_2 is illustrated in Figure 1. µ-kinetic modelling was applied to the mechanism to describe the degradation of IrO_2 under oxygen evolution conditions in both acidic and alkaline environments based on experimental degradation measurements performed by Mayrhofer *et al.* [2] and Schalenbach *et al.* [3]. The objective of the µ-kinetic model was to establish a relationship between the potential and the degradation of IrO_2, where the alkaline version was implemented into a continuum model developed by SINTEF [4] simulating the operation of an AEM-WE, trying to qualitatively capture the effects of anode catalyst degradation during polarization. To be consistent with the µ-kinetic model, it was assumed only catalyst exposed to electrolyte could undergo degradation, as illustrated in Figure 2.

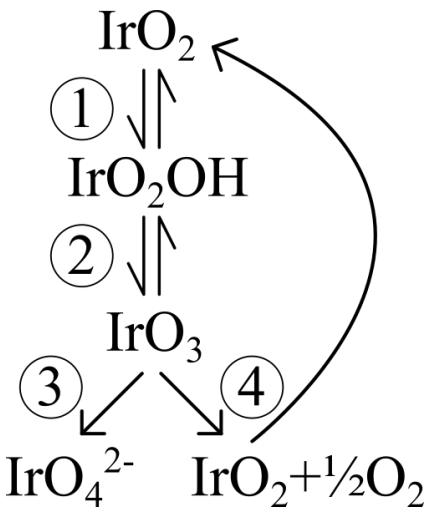

Figure 1: Reaction pathway for IrO_2 as electrocatalyst for the OER with iridium dissolution. Simplified reaction pathway inspired by Kasian et al.[1]

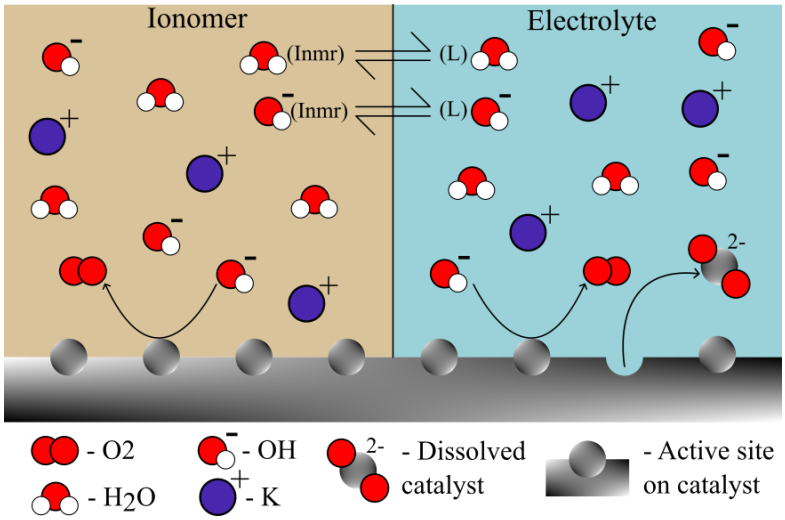

Figure 2: Oxygen evolution and IrO_2 dissolution during operation of the AEM. There is assumed no degradation for the catalyst covered by ionomer.

The simulations showed that catalyst degradation led to an offset in polarization curves, indicating a worsening in performance, but the offset was smaller than expected. Furthermore, degradation did not occur uniformly across the catalyst layer; the rate of degradation was indeed faster closest to the anion-exchange membrane. However, the alkaline microkinetic model implemented in the continuum model predicted too rapid degradation under normal AEM-WE operating conditions, suggesting a discrepancy between the continuum model and the microkinetic model. Nevertheless, the use of microkinetic modelling to qualitatively describe the effects of degradation of IrO_2 as an oxygen evolution catalyst used in an AEM-WE was successful.

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