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Transient performance modeling of photoelectrochemical cells incorporating nano-structured photoanodes SOPHIA HAUSSENER, MIKAEL DUMORTIER, EPFL — Photoelectrochemical processes constitute a viable route for renewable hydrogen production. Several practical systems that provide separated product streams of hydrogen and oxygen follow the design guidelines established in the fuel cell community and have been demonstrated. We developed a transient 1D numerical model of a photoelectrochemical fuel cell-based device, which incorporates a complex, nano-structured photoanode. The model accounted for radiation transport, charge carrier transport, species transport, fluid flow and electrochemical reactions. We investigated the transient performance under varying illumination, species mix and phases, and examined different types of nanostructured photoanodes, i.e. based on carbon-paper infiltrated with photoactive particles or carbon nanotubes uniformly covered by photoactive layers. Our model predicted the operational-dependent and experimentally observed four regimes of the transient photocurrent: anodic overshoot at illumination start, current increase, current decrease, and cathodic undershoot. The numerical results supported the hypothesis that the transient behavior of the photocurrent at startup was dominated by the low initial concentration of hydrogen and oxygen. The validated model developed provides a useful tool for system design and operational guidelines to avoid these regimes and keep the device at a stable operation and at a maximum efficiency.

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