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A PHREEQC Reactive Transport Simulation for Simply Determining Scaling during Desalination

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Abstract : Freshwater is a vital resource; yet, the supply of clean freshwater is diminishing as the consequence of melting snow and ice from global warming, pollution from industry, and an increasing demand from human population growth. The unsustainable trajectory of diminishing water resources is projected to jeopardize water security for billions of people in the 21st century. Membrane desalination technologies may resolve the growing discrepancy between supply and demand by filtering arbitrary feed water into a fraction of renewable, clean water and a fraction of highly concentrated brine. The leading hindrance of membrane desalination is fouling, whereby the highly concentrated brine solution encourages micro-organismal colonization and/or the precipitation of occlusive minerals (i.e. scale) upon the membrane surface. Thus, an understanding of brine formation is necessary to mitigate membrane fouling and to develop efficacious desalination technologies that can bolster the supply of available freshwater. This study presents a reactive transport simulation of brine formation and scale deposition during reverse osmosis (RO) desalination. The simulation conceptually represents the RO module as a one-dimensional domain, where feed water directionally enters the domain with a prescribed fluid velocity and is iteratively concentrated in the immobile layer of a dual porosity model. Geochemical PHREEQC code numerically evaluated the conceptual model with parameters for the BW30-400 RO module and for real water feed sources – e.g. the Red and Mediterranean seas, and produced waters from American oil-wells, based upon peer-review data. The presented simulation is computationally simpler, and hence less resource intensive, than the existent and more rigorous simulations of desalination phenomena, like TOUGHREACT. The end-user may readily prepare input files and execute simulations on a personal computer with open source software. The graphical results of fouling-potential and brine characteristics may therefore be particularly useful as the initial tool for screening candidate feed water sources and/or informing the selection of an RO module.

Keywords : desalination, PHREEQC, reactive transport, scaling
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