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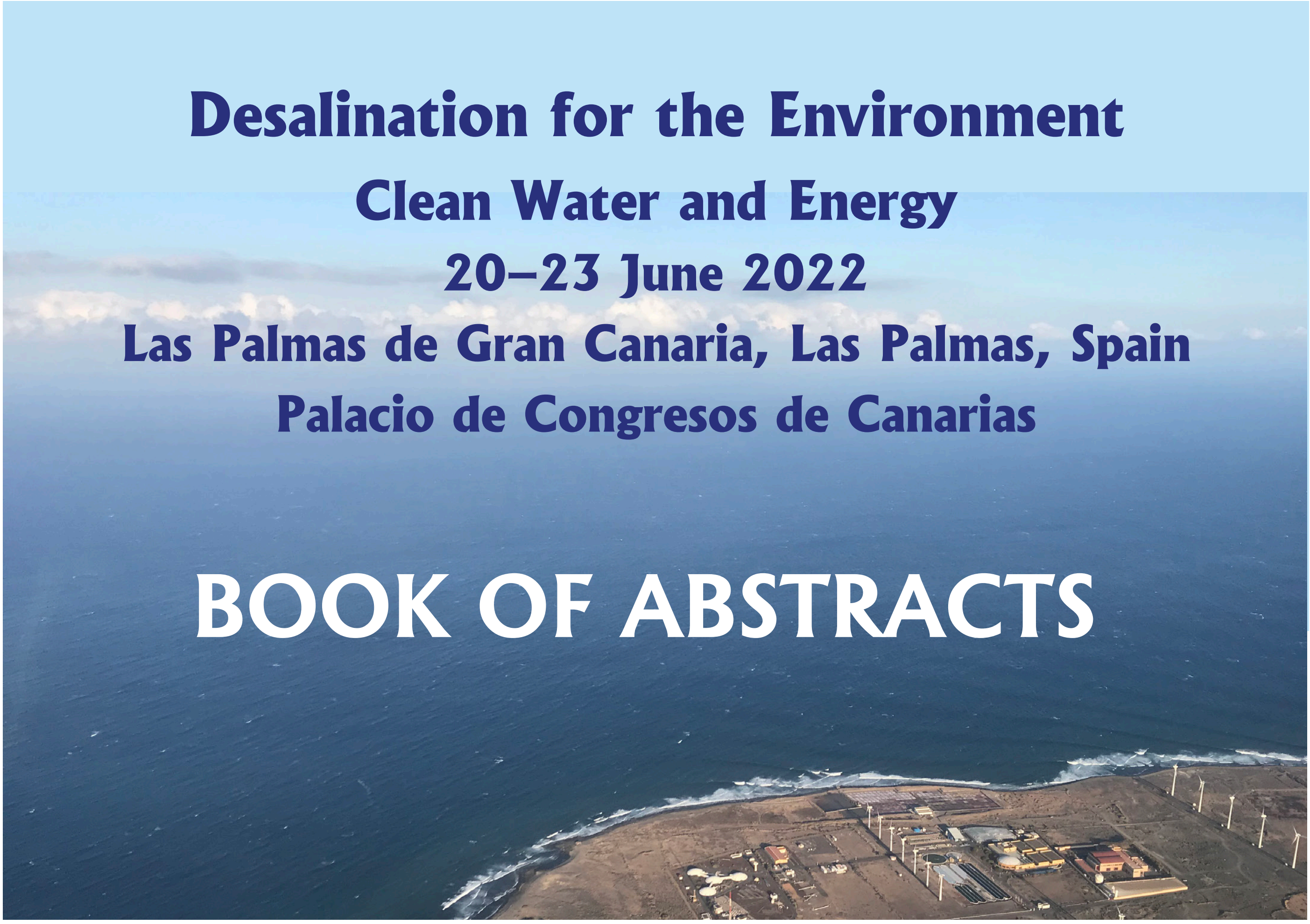
BOOK OF ABSTRACTS



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Simulation of bipolar membrane electrodialysis (BMED) units by a validated process model

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The BMED technology can be used for the production or the regeneration of acid and base solutions by water dissociation. BMED has practical applications in several fields including in chemical and biochemical industry, environmental protection and, recently, even for brine valorisation. Many are the irreversibility sources involved in the BMED process. Some of them are related to the non-ideal transport properties of the ion exchange membranes causing undesired co-ion leakages and water flux. Furthermore, the presence of shunt currents through the manifolds (i.e. distributors and collectors of the solutions) decrease the current efficiency.

The aim of this work is to give a quantitative description of the main phenomena involved in BMED processes by a multi-scale model. Four different dimensional scales were effectively combined within the gPROMS platform. The lowest scale simulates the channels and includes two sub-models. CFD simulations are devoted to the estimation of concentration polarization phenomena and pressure losses while the other channel sub-model evaluates the physical properties of the solutions. The middle-low level simulates the triplets, combining mass balance equations and fluxes through the membranes. Moreover, this model scale calculates electrical variables as the cell resistance and the electromotive force. Channel and triplet scales were implemented with 1-D discretization of the variables. The middle-high level is the stack model. It includes two sub-models: one predicts the shunt currents through the manifolds and the other one calculates the pressure losses in the whole stack. The highest level is the external circuit one, which computes the external pressure losses and the transient behaviour of closed-loop layouts. This multi-scale model was validated both by experiments with a laboratory test-rig unit and data already presented in literature. A sensitivity analysis was performed to gather useful information about the system performance by comparing current efficiency and net power density in different configurations. Simulation results show the effect of the operating variables (e.g. current density and mean flow velocity) and system geometry, highlighting the importance of the manifolds characteristics for the process efficiency. The thoroughness of this mathematical model provides a powerful tool for the design of BMED units.

Keywords: Electrodialysis; Bipolar membrane; Ion-exchange membrane; Water dissociation; Acid; Base; Modelling