Lattice-Boltzmann and Lagrange Particle Tracking methods based on porous medium X-ray Computed Tomography for analysing fluid dispersion in Flow Battery electrodes

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ABSTRACT

Lattice-Boltzmann simulations of fluid flow in porous media reconstructed by X-ray computed tomography (CT) allow to characterize the macroscopic behaviour of fluid flow and dispersion in porous electrodes for flow batteries [1]. In particular, micro-CT enables the non-destructive evaluation of internal porosity and fibers orientation with micrometric resolution [2]. In this work, metrological micro-CT has been used to obtain high-accuracy three-dimensional reconstructions of the analysed material. The obtained data have been used as input geometry in the Lattice-Boltzmann algorithm. The Lattice-Boltzmann model has been coupled with a Lagrangian Particle Tracking algorithm in order to better analyse the complex dispersion behaviour of species induced by the medium microstructure that conforms a superdiffusive behaviour [3]. Different materials have been investigated, including typical carbon felt used as electrodes in redox flow batteries and innovative carbonized rigid materials. The effects of the anisotropy due to the fibre orientation have been investigated (Fig. 1). For each material and microstructure, the flow behaviour and particle trajectories have been computed extracting synthetic flow resistance and dispersion features (Fig 2). These analyses allow identifying the optimal material and its arrangement, such as to involve minimal drag and maximized mixing. These conditions ensure increased performance of the redox flow cell, as regards reduced diffusion losses in the electrochemical reaction as well as reduced pressure drop and pumping needs of the electrolyte solutions.

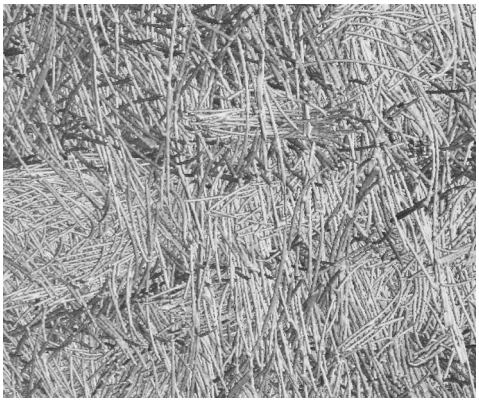

Fig. 1 µCT 3D recostruction of a carbon felt

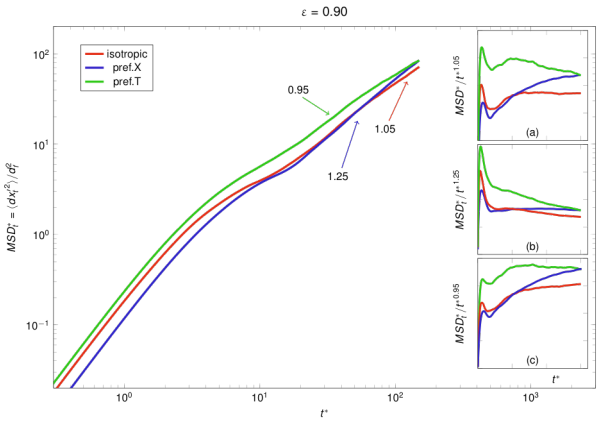

Fig. 2 Evidence of particle superdiffusive behavior

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