Joint (EE+AP) Master Project: Nanoscale analyses for macroscale models of charge transport in dielectrics

Electric field models for the insulation of the future AC/DC electric grid

The widespread of electrical processes involving DC voltages at both generation and utilization level is raising attention towards a hybrid AC/DC Medium Voltage (MV) distribution grid [1]. The insulation of the components operating in this infrastructure would experience superimposed AC+DC voltage stresses. Nevertheless, the high compactness required for MV distribution installations decreases the available design margin. Therefore, more reliable modelling of electric fields is needed.

Charge transport modelling in dielectrics

Modelling mixed AC+DC electric fields in dielectrics requires including the effects of both the dielectric polarization of the insulation and the phenomena of ionic charge transport (Fig.1). Such phenomena can be predicted with a multiphysics approach by electrohydrodynamic (EHD) models [2].

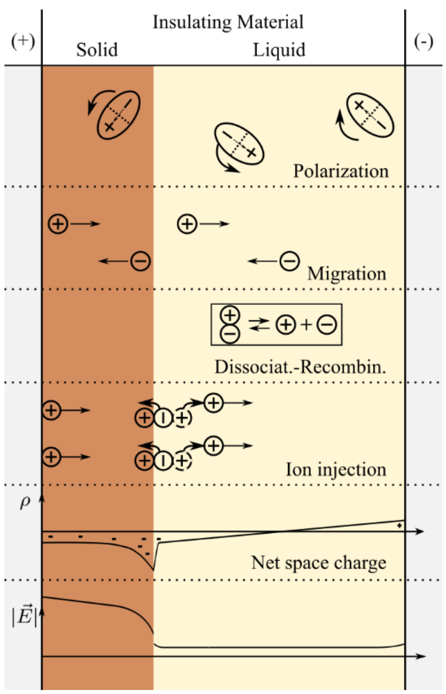

Fig. 1. Phenomenology

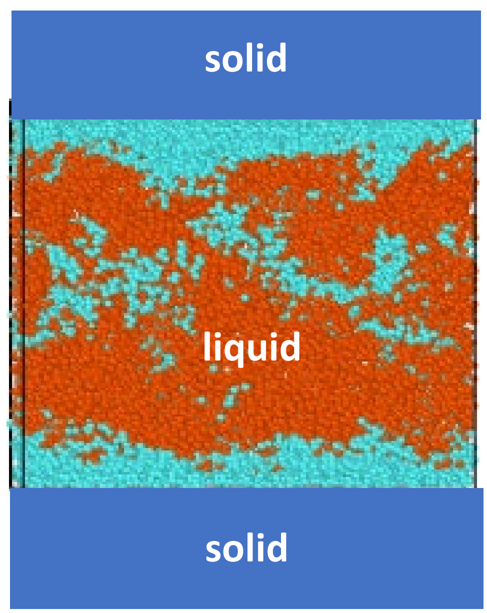

Fig. 1. Molecular-dynamics modelling of the interfaces

The physical mechanisms occurring at the interface between different materials are still unclear, and the boundary conditions used in the EHD model sometimes rely on fitting the data measured from experiments on simple geometries [3].

In this project, the candidate will investigate the applicability of atomistic computer simulations of ionic transport at nanoscale level (Fig.2), to support the formulation of suitable boundary conditions in EHD models. The atomistic modelling of the solid-liquid interfaces, Fig. 2, will be carried out by classical molecular-dynamics simulations. The exact chemical structure of participating materials will be taken into account. The ion diffusion, the structure of the charged layers at the interfaces will be calculated. The simulations will be performed with highly-optimized LAMMPS and/or Gromacs molecular-dynamics packages.

Assignment

The assignment consists of:

1. Investigate the applicability of atomistic computer simulations for determining the ionic properties of a dielectric material;
2. Nanoscale analysis of the interfacial phenomena;
3. Post-processing of the atomic scale modelling for macromolecules; formulation of proper boundary conditions to utilize for modelling charge transport at macroscopic scales.
4. **Optional**: Experimental verification

Supervision: EPE group (Electrical Engineering, Dr. M. Curti, MSc. A. Cremasco), with co-supervising of TPS group (Applied Physics, Dr. A. Lyulin)

The EPE group has one of the most advanced electro-mechanic and power electronics laboratory in the Netherlands (680+ m^2 floor space) and contains state of the art facilities for testing and validation of electro-mechanic and power electronic systems. This laboratory is supported by 5 technicians. There is a strong connection with industry, underlined by our 15 part-time fellows, and the job opportunities are numerous. The research is challenging, with subjects that include, for example, ultra-high precision systems, modelling and optimization techniques, advanced scalable power electronics, and special rotary machines such as high-speed machines. The capacity group currently consists of 2 full professors, 2 associate professors, 5 assistant professors, >20 PhD students and 5 technicians.

The TPS group will supervise the computer simulations part of the planned research.

References

[1] G. F. Reed, B. M. Grainger, A. R. Sparacino, E. J. Taylor, M. J. Korytowski, and Z. Mao, “Medium Voltage DC Technology Developments, Applications, and Trends,” in *CIGRE US National Committee 2012 Grid of the Future Symposium*, 2012.

[2] M. Tefferi, M. Ghassemi, C. Calebrese, Q. Chen, and Y. Cao, “Correlation between current-voltage characteristics and DC field grading for dielectric liquid used in wet-mate DC connector,” IEEE Trans. Dielectr. Electr. Insul., vol. 25, no. 5, pp. 1668–1678, 2018.

[3] A. Denat, “Conduction and breakdown initiation in dielectric liquids,” Proc. - IEEE Int. Conf. Dielectr. Liq., July, 2011.