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Advancing the Open Electromagnetic Modeling Platform for Electrochemistry and Energy Materials

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ABSTRACT

This paper highlights recent advancements in Open Innovation Environments within the scope of European Union research initiatives. It introduces an extension to an open-access computational electromagnetics platform, enabling the modeling of coupled electrochemical processes at electrolyte/electrode interfaces. The solution integrates Laplace/Poisson equations with drift-diffusion equations, forming a fundamental framework for simulating ion transport in electrolytes, such as those in Li-ion batteries. A coupled FDTD solver has been developed and validated against analytical electrostatic solutions and independent FEM-based electrochemical models. This tool is designed for open usage, particularly in modeling industrially relevant battery material test setups, like those in the H2020 NanoBat project.

Keywords: computational electromagnetics, computational chemistry, coupled process modelling, open modelling platform, open innovation environment, FD method, and FDTD method.

INTRODUCTION

For many years, electrical engineers have relied on computational electromagnetics (CEM) as a fundamental tool for precisely modelling intricate electromagnetic fields and processes. The CEM must be combined with other physical models, nevertheless, because of the variety of industries that are available and the increasing complexity of connected issues. With the advent of microwaveable food packaging and the conventional FDTD (Finite-Difference Time-Domain) extending requirement in the early 2000s, this necessity became particularly clear. In order to improve the model's depiction of how microwaves interact with food, these additions added additional physical phenomena, such as heat conduction and heat capacity dependant properties of the materials under study. This innovation demonstrated how the CEM's requirements may be tailored to the needs of the corresponding industry.

Similarly, a far more sophisticated approach is needed for energy materials, particularly those utilized in batteries and photovoltaics. For precise modelling and analysis of these materials, the conventional CEM framework needs to be expanded to account for charge transport pathways. For instance, in order to explain ion mobility, voltage, and battery performance, coupled electrochemical processes must be taken into consideration for lithium-ion (Li-ion) batteries, which are frequently used for energy storage in portable gadgets and electric cars.Without integrating charge transport models, such simulations would lack the necessary precision for effective design and optimization.

To address these challenges, our work extends traditional EM FDTD tools by integrating drift-diffusion models, which simulate the movement of charged particles in an electric field. This extension was carried out within the framework of European Horizon 2020 projects, which emphasize Open Innovation. By adopting an open-access approach, we aim to make these advanced simulation tools available to the broader scientific community, as well as to industry stakeholders, promoting collaboration and accelerating innovation.

The extended platform merges reduced-power versions of commercial CEM tools with new models specifically designed for material testing, particularly in the context of energy materials. These tools are made accessible through a user-friendly, license-free graphical interface, enabling users to easily apply various electromagnetic and multiphysics solvers for their research. This paper details the new capabilities of the EM FDTD platform, specifically its ability to simulate charge transport processes. Section II outlines the key equations driving these simulations, Section III presents benchmarking examples to validate the approach, and Section IV concludes with a discussion of the platform's potential for future research and industrial applications.

Physical Model

We model a 2D electrolyte region polarized by fixed-potential electrodes, focusing on the electric potential, electric field, charge distribution, and drift-diffusion currents over time and space.

A. Electrostatics

The electrostatic model determines the electric potential (U) using:

1. **Electric Field**: $E = -\nabla UE$
2. **Charge Density**: $\nabla \cdot D = \rho$
3. **Poisson Equation**: $\nabla^2 U = -\rho/\epsilon$
4. This system is solved iteratively until convergence.

B. Drift-Diffusion Model

This model incorporates ion flow governed by drift and diffusion:

$J^+ = \mu^+ \rho^+ E - D^+ \nabla \rho^+$

$J^- = -\mu^- \rho^- E - D^- \nabla \rho^-$

Charge distributions evolve over time using continuity equations:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot J = 0$$

C. Discretization

The FDTD method, adapted from [12], is used for numerical solutions. Physical quantities are staggered in a grid to ensure second-order accuracy. The iterative updates ensure charge conservation and solution stability.

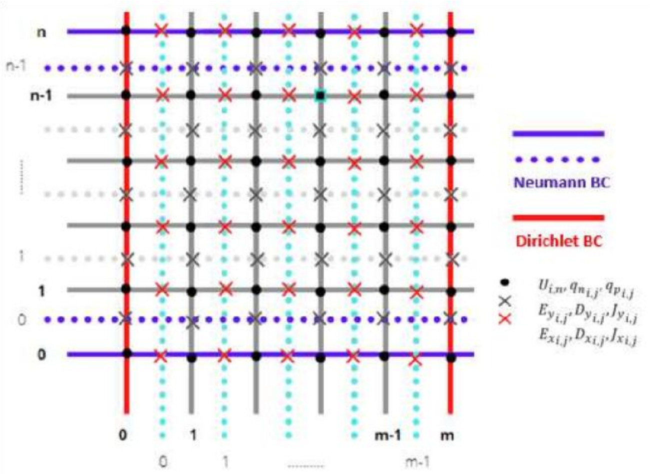

Fig.1. Staggered mesh utilized for the FDTD solution of Poisson equations coupled with Drift-Diffusion equations.

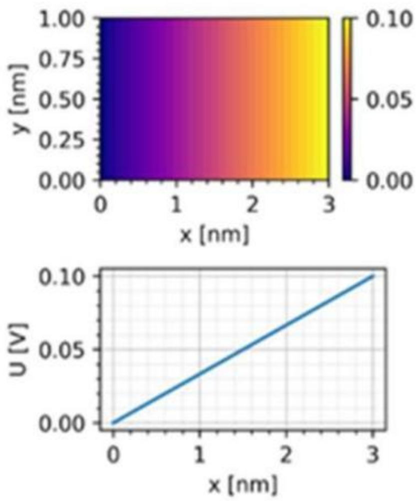

Fig. 2. Distribution of electric potential (U) in a 3 nm region containing a non-ionized electrolyte with a relative permittivity (ε_r) of 2.82, bounded by electrodes with a 0.1 V potential difference.

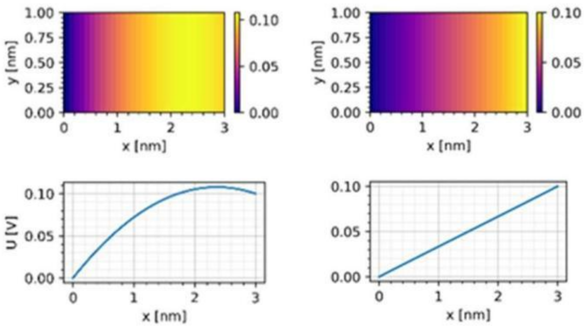

Fig. 3. Electric potential (U) distribution in a 3 nm region, bounded by electrodes with a 0.1 V potential difference, containing an electrolyte with a relative permittivity (ε_r) of 2.82 and static charges at a molar concentration of 10 mol/m^3: (left) only positive ions, (right) both positive and negative ions.

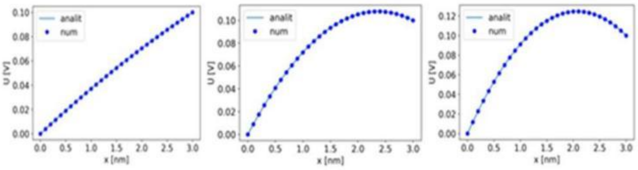

Fig. 4. Electric potential (U) distribution in a 3 nm region, bounded by electrodes with a 0.1 V potential difference, filled with an electrolyte of relative permittivity (ε_r) 2.82 and static positive charges at molar concentrations of: (a) 1 mol/m3^33, (b) 10 mol/m^3, and (c) 15 mol/m^3.

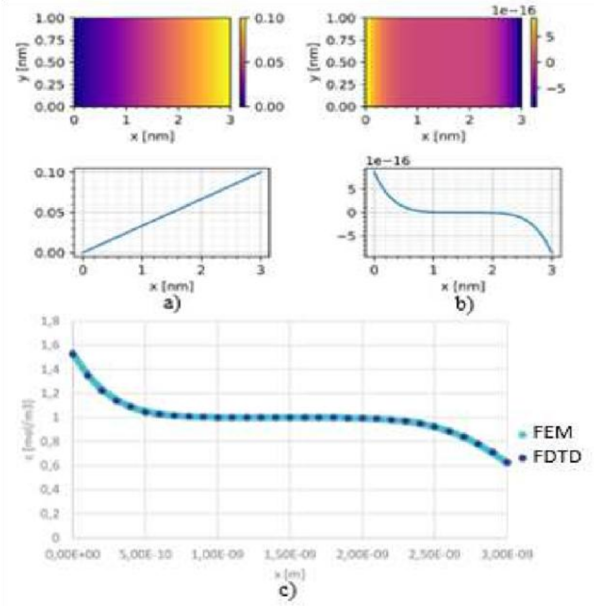

Fig. 5. Distributions of electric potential (a), total charge (b), and positive charge (c) in a region bounded by electrodes with a 0.1 V potential difference. Dc = 10−9m2/s is the coefficient of diffusion of counter ions in an electrolyte with a relative permittivity (εr) = 2.82 and initially uniformly dispersed positive and negative ions at a concentration of 1 mol/m^3.

While the potential difference between the electrodes is assumed to be 0.1 V, the following parameters are studied in a region defined by borders carrying the electrodes: electric potential, total charge, and positive charge. An electrolyte with a relative permittivity of 2.82 fills this area, and each ion's initial charge density is equal to and opposite to 1 mol/m^3. The ions are considered to have a diffusion coefficient of 10−9 m^2/s. These included the distribution of the electric potential (a), the distribution of the total charge (b), and the distribution of the positive charge (c) in this area. The findings show how the electric potential and charge concentration alter in a drop's geometry based on the electrolyte's initial ion concentration and diffusion coefficient properties in both space and time. This information will be used to forecast how the electrolyte will behave in the future when an electric field is applied.

Examples

Using the generated FDTD code, three models were examined in this work. Each model had planar electrodes inserted in the 3 nm region, with the bottom electrode grounded and the top electrode at 0.1 V. The Laplace equation was solved and compared to the expected value for a parallel-plate capacitor in the first model, which looked at electrostatics. The match was perfect. The second kind of model used uniform charge distributions throughout the area to solve for static charges. The findings demonstrated how the potential distribution's nature shifted from linear to parabolic and how much it altered in response to charge density. This change effectively illustrated how static charges affect a system's electrical potential. Last but not least, the third model made advantage of drift-diffusion, which allows the ions to travel and spread throughout the gel matrix. Here, the ions' movement through the electrolyte under the influence of the applied electric field caused changes in the charge and potential distributions over time. The use of the FDTD solver in the modelling of these electrochemical processes was validated when the steady-state solution produced by this model was compared to that obtained from a Finite Element Method (FEM) simulation carried out using COMSOL software. The results demonstrated complete conformance to one another.

CONCLUSIONS

By expanding its functionality to depict the processes resulting from electrochemical interactions in energy materials—which are common in batteries and other energy storage technologies—this work enhances an open-access simulation tool that already exists. A reference Finite-Difference Time-Domain (FDTD) solver that effectively resolves the coupled Poisson and Drift-Diffusion equations is included in the platform. The electrostatic interactions between charged layers and the movement of ions in electrolytes, which are crucial in electrochemistry, can be replicated by this solver. These findings have been confirmed by comparison with Finite Element Method (FEM) solutions for more complicated electrochemical scenarios as well as analytical answers for comparatively basic cases.

The platform's multiphysics extensions will be improved in future development to enable even more thorough simulation of the interactions between different physical processes in energy materials, such as mechanical stress or heat transfer. Additionally, these improvements will guarantee that the platform is at the forefront of electrochemical and energy materials research. The platform will continue to be accessible to both academics and practitioners, and it will encourage multi-sector involvement in accordance with the core tenets of the ER open research policies. Thus, this strategy promotes creativity and accelerates technological advancement in the field of energy materials.

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