

Three year postdoctoral or doctoral position at Humboldt University of
Berlin, Department of Mathematics, Berlin, Germany

NANO-COATED METAL FOR BIPOLAR PLATES OF PEFC: MODELLING AND SIMULATION OF MULTI-SCALE EVOLUTION EQUATIONS

Advisorship :

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Financial Support

The post-doctoral or doctoral position will be supported by an BMBF project (Federal Ministry of Education and Research) and the gross wage will be about 4000 Euro per month for a period of 36 months (BAT II A East), i.e. starting with one year with the possible extension to another one.

1 Context of the Study

The polymer-electrolyte-fuel-cell systems (PEFC) are constructed with the use of metallic bipolar plates. The corrosion of the metallic plates are a main problem in the fuel-cell system, therefore it is important to have a corrosion-resistant coating. In this project, we simulate the coating process of the metallic bipolar plates. The model equations are multi-scale evolution equations, e.g. convection-diffusion reaction equations, to simulate the coating process, see [4]. Because of the different scales, we deal with stiff partial differential equations and decomposition methods are important to solve the problem, see [1], [3]. The application of scale-decoupling algorithm are needed. A further question is based on the application of the correct model, because of very low pressure, the Boltzmann-equations are necessary to model the situation. Here the comparison between Boltzmann and Navier-Stokes, here we want to see the applicability of such continuum model. Simulation of scenarios are done with different geometries, that are used for the bipolar plates. Such parameter studies allow to have results for the physical experiments.

2 Simulation of the Coating Process

2.1 Objectives of the study

The objective of the post-doctoral or doctoral position are threefold. First the understanding of the model problem and the usage of the academic program-tools are important. Then, some first applications are performed with the underlying software-codes. Here, the candidate have to implement the underlying geometry and parameters of the model. Finally the implementation of decoupling methods are done to see the benefit of such scale dependent algorithm and real-life simulations should be done.

2.2 Applications

The study of the underlying chemical structure, see [5], with complex chemistry is important and these structures should be simulated. Based on the advection and diffusion process of the gas with the coated material, the structure of the material surface has to be studied. For first test examples the equations are implemented via MATLAB and the results are compared with physical experiments. In a next step, the applications can be implemented in academic program-tools, e.g. UG, ADINA, DUME, etc. . With such codes, real-life simulations in 2d and 3d are possible. Error estimates and decomposition methods can be implemented to accelerate the computational time.

3 Necessary Background

Numerical analysis (Partial differential equations). Scientific programming and computing (MATLAB, C, C++). Interest for applications in the field of physics and chemistry.

Literatur

- [1] I. Farago, J. Geiser. *Iterative Operator-Splitting Methods for Linear Problems*. IJCS, International Journal of Computational Sciences, accepted, June 2005.

- [2] J. Geiser. *Discretization methods with analytical solutions for convection-diffusion-dispersion-reaction-equations and applications*. Journal of Engineering Mathematics, published online, Oktober 2006.
- [3] J. Geiser. *Iterative Operator-Splitting Methods with higher order Time-Integration Methods and Applications for Parabolic Partial Differential Equations*. Journal of Computational and Applied Mathematics, Elsevier, accepted, June 2007.
- [4] J. Geiser. *Discretisation methods for systems of convective-diffusive-dispersive-reactive equations and applications*. Doctor Thesis, University Heidelberg, Germany, 2004.
- [5] T.K. Senega and R.P. Brinkmann. *A multi-component transport model for non-equilibrium low-temperature low-pressure plasmas*. J. Phys. D: Appl.Phys., 39, 1606–1618, 2006.