Proposal for Young Scientist IAPWS project

for the year of 2006 in the course of 5 months.

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Irreversible thermodynamics of fuel cells membrane transport

Hydrogen/oxygen fuel cells based on the reactions of oxidation of H_2 and reduction of O_2 ($2H_2 + O_2 = 2H_2O$) represent a prospective alternative to traditional ways of generating electrical energy. Since electrical energy can easily be converted into mechanical energy, the fuel cells are also strong candidates for replacing combustion engines, e.g. in vehicles. The basic principle of a fuel cell has been known for about 150 years and it is sometimes referred to as ”reversed electrolysis”. In a so-called proton exchange membrane (PEM) fuel cell, two electrodes are separated with an electrolyte, which is a very thin (no more than a few tens of micrometers) membrane made of a proton conductive polymer (e.g. Nafion). At the anode hydrogen is oxidized, producing protons and electrons. The electrons flow through an external circuit, while the protons must pass through the electrolyte membrane. At the cathode the electrons and the protons react with supplied oxygen to form water. The electrodes are attached to the membrane forming the so-called membrane electrode assembly (MEA).

Transport processes occurring in MEA are considered to be a crucial point of the fuel cell operation and efficiency. Several models describing these processes have been developed thus far. Some of them focus only on a selected part of PEM fuel cell, while others attempt to describe the behavior of the whole cell considering it as a black box. In this project we would like to focus on the investigation of a possible influence of the membrane material, membrane geometry, and other parameters such as, pressure, temperature, humidity, etc. Due to strong concentrations of protons and electrical field gradients, the application of the extended non-equilibrium (irreversible) thermodynamics is desirable. In the frame of this theory it is possible to include all relevant processes like

convection, diffusion, heat transfer, ionic conductivity, and electrochemical reactions in a natural way, i.e. based on the entropy production concept.

The expertise of the host, The Pennsylvania State University (Penn State), will be of great advantage for the applicant in selecting and modifying an appropriate model and, especially, to supply necessary experimental data. The research team of The Energy Institute's Electrochemical Laboratory at Penn State under the direction of Dr. Lvov has long-term expertise in PEM fuel cell research and high-temperature electrochemical studies. Current experimental systems cover a complete range of membrane and powder tests, including high-temperature proton conductivity (using Electrochemical Impedance Spectroscopy), water uptake, high-temperature electrophoresis for electrokinetic studies of inorganic particles, membrane casting and membrane-electrode assembly (MEA) preparation, high-temperature membrane permeability, and high-temperature fuel cell performance. Research projects on high-temperature PEM fuel cells are carried out with support of Department of Energy, Oak Ridge National Laboratory, and DuPont.

The aims of the project.

1 Prepare a database of existing physico-chemical models describing transport and electrochemical processes which occur at all components of MEA of PEM hydrogen/oxygen fuel cells.
2 Formulate an adequate physico-chemical model describing the influence of membrane material, including composite materials on the PEM fuel cell performance.
3 Develop a computer program for numerical simulations of the model and investigate the behavior of the model in a series of simulations.
4 Compare the results of numerical simulations with available experimental results and possibly improve the original model, so that it yield a better agreement with the experiment.

The stay of Ondřej Mičan at The Pennsylvania State University will be supervised by Dr. Serguei Lvov who is an expert in the field of electrochemistry and PEM fuel cells. O. Mičan will spend the proposed 5 months with Dr. Lvov in his lab at Penn State. It is proposed to start Ondřej Mičan's visit in February 2006.

Budget:
A round trip from Prague to State College: $2,000
Per month in State College: $1,500 * 5 = $7,500
Total: $9,500

Attachment: Mr. Ondřej Mičan's Curriculum Vitae

Attachment 11

CURRICULUM VITAE

Personal Details

Name:	Ondřej Mičan
Address:	Kaplická 57 140 00 Praha 4 The Czech Republic
Date of birth:	19th December 1977
Place of birth:	Prague, The Czech Republic
Title:	Ing.
Marital status:	Single
Nationality:	Czech
Telephone:	+420 604 627 004, +420 723 682 691
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Education

1984 – 1992	Elementary school in Prague.
1992 – 1996	Electrotechnical high school in Prague. Specialization: Electronical Computer Systems.
1997 – 2003	Czech Technical University in Prague, Faculty of Nuclear Science And Physical Engineering. Specialization: Mathematical Modeling. *Diploma thesis: Chaotic Dynamics of Reactiondiffusion Equations.*
Since 2003	PhD. study at Czech Technical University in Prague, Faculty of Nuclear Science And Physical Engineering. Specialization: Mathematical Modeling.

Work Experience

2001	Mediatel, s. r. o., entering data into a database.
Since 2002	Unicorn, a. s., programmer, analyst.
Since 2003	FNSPE, CTU Prague, teaching (calculus, algorithms).

Skills

Foreign languages:	English (very good knowledge), German (basic knowledge)
Programming languages:	C++, Perl, Java, PL/SQL, JCL,……
Driving licence:	personal vehicles

Hobbies

Music:	playing the guitar, singing.
Sports:	bicycle, rollerskates, volleyball, . . .