Research project objectives/ Research hypothesis

The proposed project is focused on theoretical and experimental studies of processes occurred during steam reforming of hydrocarbons internally at the anode of Molten Carbonate Fuel Cell (MCFC). The main objective of the project is to develop a novel description of processes of the electrochemical conversion of methane to hydrogen at anode fuel cell conditions. Due to the nature of the modus operandi of MCFC and the steam reformer of methane, these studies are interdisciplinary in nature, taking into account the phenomena of electrochemical, catalytic, and the exchange of mass, energy, and electric charge.

The aim of the project is to investigate and demonstrate the electrochemical processes of supplying steam to reaction of decomposition of methane to hydrogen in the reactor created in the anode of MCFC and developing appropriate mathematical models describing these phenomena. We propose a research hypothesis, which involves the ability of independent work of reformer on anode of MCFC. It is expected that the models will allow the development of a cell which can support the appropriate level of reforming conversion to allow for the separation and identification of the influence of individual factors on the composition of the gas at the outlet of the anode. In addition, it is possible that electrochemical supplying of steam (via oxidation of hydrogen) can lead to an intensification of reaction and improved thermal management of anode channel. It should be emphasized that the processes which are the subject of the proposed project have not been practically tested so far and it is not possible to find any estimates about the feasibility of such a hybrid reaction.

Research project methodology

The methodology of proposed project involves a combination of experimental techniques and mathematical modeling. The modeling will be used to design experiments and build a test stand for electrochemical measurements. Experimental studies are planned to enable confirmation or denial of the research hypothesis and to provide data for numerical models. These models will allow to identify the key processes that occur on a common anode channel along a porous electrode of MCFC and on the catalyst in the form of pellets or balls disposed on the current collector in high temperature, and to determine the appropriate working conditions of such a reactor. In order to determine potential applications and make appropriate calculations and simulation optimization it is necessary to build appropriate mathematical model of this phenomenon. In the previous solutions, fuel cells could be supplied with hydrocarbons using an external reformer. The applied research methodology will be based on mathematical modeling and digital simulation supplemented by tests on laboratory stand. An own computer software and commercially available (AspenPlus, HYSYS and/or GateCycle) will be used. The authors of the proposal have access to this software and required skills. Detailed simulation studies by own and commercial codes will be carried out. It will include the preparation of consistent models, which implies the use of models in the same class for all analyzed devices.

The project provides for the following tasks: 1. Development of numerical models enabling analysis of phenomena occurring during steam decomposition of methane on the fuel cell anode - study of the influence of catalyst parameters on reaction rate; 2. Development of discrete kinetic response models for analysis of the anodic side of the cell in the full load range - determination of the influence of the catalyst geometric parameters and current collector on the characteristics of the processes under way; 3. Experimental studies for selected variants of catalyser vs. current collector in full load cell range - determination of cell characteristics and determination of limit load; 4. Validation of developed numerical models with experimental results; 5. Analysis of exhaust gas compositions for individual variants enabling assessment of the catalytic reaction rate of critical operating conditions of the cell; 6. Analysis and development of research results.

Expected impact of the research project on the development of science, civilization and society

Within the project a mathematical model of the process of steam reforming of methane inside the MCFC fuel cell stack designed to test and simulate the dynamics of this phenomenon will be developed.

Implementation of the project concerns on the basic research, which are the key to understanding the chemical and physical processes occurring in high temperature, electrochemical devices. The achieved results will help determine the possibilities which brings a hybrid of MCFC and steam methane reformer to high temperature decomposition of natural gas to hydrogen in electrochemical processes. This knowledge will form the basis for further development of fuel cell technology – conversion of chemical energy of fuel directly into electricity. This will broaden the knowledge on the phenomenon described above. These results can be used in the future to facilitate the use of natural gas to supply the high-temperature fuel cells.