Abstract of PhD thesis

„**Numerical modelling of power generation systems based on fuel cells using process simulator tool**”

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One of the future technology for producing electricity is fuel cell that converts the chemical energy of fuel directly into electricity. The efficiency of the direct conversion might be around 47 [%]. Cogeneration systems based on Solid Oxide Fuel Cells operate with an efficiency of even 85 [%]. It should be noted that a significant operating temperature of the Solid Oxide Fuel Cell (SOFC) may cause problems with thermal expansion of cell structures whose thickness is the order of micrometres. To determine and maintain optimal operating conditions for a single cell as well as a stack and other components, which are part of the systems for the production of electricity and heat, the use of modern and innovative research tools as process simulator is required. The results of numerical simulations, on the one hand, allow to significantly reduce the costs of the design and laboratory testing, and on the other hand, allow to consider a much larger number of operational parameters influencing the operation of these systems in a shorter time.

Taking into account the above, it was decided that the aim of the dissertation was to carry out numerical modelling of power generated systems equipped with high temperature Solid Oxide Fuel Cells at the steady state and transient state using a modern design tool represented by a process simulator. The dissertation was divided into seven main chapters.

The first chapter includes a brief introduction to the analyzed issues covering the characteristics of fuel cells and basics of the modelling of systems based on fuel cells using a process simulator. Weaknesses and strengths of the research tool have been identified.

The second chapter contains a summary of the state-of-the-art on the application of the process simulators to the modelling of systems equipped with SOFC for the generation of electricity and thermal energy. In order to better understand the issue,

a review of basic types of fuel cells and their specifications was performed. Components of the complete power system were described and the operation of a process simulator was presented. The summary of the chapter is a description of conclusions drawn on the basis of the conducted literature review. A research gap has been identified, the filling of which may contribute to science development. The outcome of the literature review was the formulation of detailed goals and research theses of the doctoral dissertation, which are presented in the next chapter.

Chapter three covers a key purpose of the dissertation, namely the modelling of mass, energy transport and electrochemical reactions within a system for the generation of electric energy and heat equipped with two stacks of high-temperature ceramic Solid Oxide Fuel Cells of different number of cells in each stacks by means of a process simulator. An additional aspect of the novelty was the application of two separate fuel reforming subsystems. Achieving the assumed goal forced the definition of detailed objectives. The detailed objectives finally allowed to achieve the main objective and were implemented in stages.

A description of the work carried out is presented in Chapter 4 showing the own research. As part of the first stage, preliminary research was conducted, which resulted in defining in a process simulator a mathematical model in the steady state for a simple power supply system containing a single stack of SOFCs. The system was named as system A. A set of mathematical equations was also defined allowing to estimate the current-voltage characteristic of a single cell for various values of operational parameters. The obtained results of numerical simulations for the I-V curves were compared with the available measurement data and the results were found to be in accordance at the acceptable level. The next stage, after verifying the correctness of the modeling predictions, a numerical analysis of the system A in the transient state was started. This required redefining the mathematical model of the power supply system operating in this case under transient conditions. Confirmation of the compatibility of the simulation results for the power supply system described as the system A in both steady state and transient state was the starting point to develop the mathematical models in steady state and transient state for the system consisting of two SOFC stacks called as system B, shown in the main research. The accuracy of the defined mathematical models was confirmed by comparing the simulation results with literature data and data obtained from partners from the European project with acronym STAGE-SOFC. This chapter closes with the presentation of the results of analyses of the impact of selected operational parameters on the performance of both systems. The carried out numerical simulations resulted in the current-voltage characteristics for SOFC stacks operating under different system loads. The analyses of such issues as the performance of power supply systems that operate at a variable fuel consumption factor and different values of molar ratio of reagents were carried out. The numerical analyses were carried out in order to determine the optimum operating conditions for simple system A and complex power supply system B.

Chapter five shows summary and concluding remarks. Based on the analysis of own results, it has been shown that the use of the process simulator can be successfully applied to predict individual operating parameters of power supply systems based on SOFC stacks both to optimise and to study the behaviour of the systems under boundary conditions. A dynamic model has been successfully defined for both power supply systems, i.e. system A and system B, respectively, together with the implementation of appropriate mathematical equations enabling calculation of the current-voltage characteristic of the SOFC cell. Based on the conducted tests, it was found that an increase in pressure and temperature in the cell had a positive impact on the amount of generated power density, and it has been shown that the temperature of the stack had a greater impact than the pressure. In the case of system B, it was found that the similar voltage values of a single cell in both stacks did not occur over the entire current density range, but as it increased, the difference increased due to a significant voltage drop in the second stack. Finally, new areas were indicated that should be the subject of further research.

Chapter six contains the references, while chapter seven presents the author’s own publications. Attachments A and B contain numerical codes for the calculation of current-voltage characteristics of fuel cells in dynamic models for system A and system B, respectively.

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