In the twentieth century, oil has played an extremely significant role, being the driving force for the development and stimulating global economies. However, nowadays the global demand for accessible and cheap energy sources still increases. Therefore, the significances of alternating fuels and emerging technologies which can prove the novel solutions for the increasing energy demand are the most urgent issues of the modern society. Natural gas, one of the commonly used fossil fuel supplementary to oil today, is nowadays playing a certain significant role in energy demand and is a promising fuel resource for the future of our economy. It is directly used in energy market or can be used to produce chemical product; further it can be a source of hydrogen production in future. To promote and economize its applications, the proper pathways to enable transportation and fluent incorporation to energy systems are necessary.

Fuel cells are emerging technology for many applications, mostly commonly studied as power source for mobility and stationary. The advantage of using fuel cells is regarded with its mechanism of producing electricity. The fuel cells produce the electricity by electrochemical conversion of hydrogen directly, which promises a high energy conversion rate with minimum loss. Hydrogen production from natural gas can be incorporated with fuel cell technology. Hydrogen production from natural gas or hydrocarbon yields carbon monoxide (CO). Proton transferring fuel cell cannot count it as fuel, and what is worse, CO can poison the electrode of those fuel cells which often adopt platinum as a catalyst. The use of expensive noble catalytic metals is related a low activity of those fuel cells at a low operating temperature, at which the functionality of fuel cell membrane are assured.

Solid Oxide Fuel Cells (SOFCs) can potentially count on the synthesis gas from natural gas regarding the electrochemical principle of transferring oxygen ion through an electrolyte at a highly elevated temperature (600-1000ºC). This enables fuelling an SOFC with CO, the so-called fuel flexibility. SOFC systems, with their high operating temperature, fuel flexibility and simplicity of the connection with a city-gas infrastructure, advertise their potential and promote themselves to have numerous application possibilities in different sector of industrial fields. As the devices, which directly convert the chemical energy of fuel into electricity, they have the potential to be economically competitive technology that can provide higher electrical efficiency in comparison to the commonly used solutions. One of the most urgent research topics in the field of SOFCs is improving their fuel flexibility to enhance their competitiveness. The high temperature fuel cells enables reforming of fuel in the internal system configuration. The design and optimization of an indirect internal reformer or a cell with direct reforming on the other hand involve many technical problems. Numerical modelling of phenomena occurring in an SOFC can be a helpful attempt to contribute the actual design and optimisation. In this context, proper kinetics of the methane/steam reforming reaction is one of the most important factors to improve the reliability of numerical results of the reforming coupled SOFC.

The kinetic of the methane/steam reforming was widely studied in the literature for the industrial catalytic reactors, however there are significant disagreements found among published data. Also, the properties of the typical industrial catalyst and SOFC dedicated materials are different, though both of them are nickel based. Therefore, the widespread disagreements between kinetic of the reforming proceeded on the typical industrial catalysts and lack of suitable kinetic on real SOFC anode materials, induce the necessity for the reliable data dedicated for SOFC design. It is crucial in the context of the great influence of the implemented reforming kinetic model for the properties and performance of the overall SOFC unit model.

This research aims to provide comprehensive description of the methane/steam reforming process dedicated for Solid Oxide Fuel Cell with respect to the uncertainty of the postulated empirical process equations and propose an objective mathematical strategy for the quality evaluation of imposed numerical models. It is postulated that the Generalized Orthogonal Least Squares method (also known as the Generalized Least Squares: GLS) can be applied to analyse, quantify and improve the mathematical modelling of methane/steam reforming process.

The first comprehensive formulation of the Least Squares method can be found in Legendre’s works and initially it was used in surveying problems and geodetic calculations and then was applied to astronomy and scientific problems. The least squares method is a basis of the modern errors theory and it is called the automobile of the modern statistical analysis. One of the most spectacular examples of the application of this mathematical theory is the discovery of binary pulsar and development of relativistic gravity theory, presented by Hulse and Taylor. The Orthogonal Least Squares Method was used as the basis of all of the calculations and the discoveries were awarded by Nobel Prize in Physics in 1993.

The proposed methodology for the analysis of methane/steam reforming process allows for including additional data directly into a mathematical model of the process as the new (supplementary) variables. The GLS method is proposed as a method of correcting the measured data, securing its higher accuracy and obtaining the most probable value and its uncertainty for the parameters to be determined by numerical computation. Additionally, the proposed method provides the objective criteria for the formal evaluation and falsification of different mathematical models of investigated phenomena.

Therefore, the GLS method can be extremely useful method for analysing the kinetic of non-equilibrium chemical processes. The preliminary research of the author of proposed study gave the promising results in the terms of improving the quality of modelling. The advantages of such approach enables for more general analysis of the problem and providing more precise information about obtained results, which includes their uncertainty. However, the systematic approach to study of the kinetic of non-equilibrium problem by the means of the falsification study of the various kinetic models by the GLS method is necessary. Therefore the proposed research will introduce a novel quality in the considered field and create a benchmark in the assessment of the quantification of the reaction kinetic studies. Also, the application to the methane/steam reforming process will be highly usable for design and optimization of SOFC system and reforming reactors.

All of the proposed numerical studies will be based on the experimental investigations. Nickel catalyst Ni/YSZ (both: commercial and prepared), which are the popular material for high temperature Solid Oxide Fuel Cells, will be used. The experimental studies for investigation of the kinetic of the methane/steam reforming will be conducted in the plug-flow reactor filled with powder catalyst. The average diameter of catalyst particle will be ~1μm, what eliminates the influence of the mass and heat transfer phenomena. The obtained experimental data will be used in numerical analysis to quantify the influence of experimental accuracy on deriving the reaction kinetics of the methane/steam reforming using the GLS method.