## Modeling of a Biogas Steam Reforming Reactor for Solid Oxide Fuel Cell Systems

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## **Abstract**

Introduction: The absence of a hydrogen refuelling infrastructure and the problems concerning hydrogen storage, has led to the development of fuel processors able to convert available fuels into hydrogen rich reformate gas. The choice of a suitable fuel processor and fuel, during the transition phase to a hydrogen economy, are the key aspects to the successful implementation of direct-hydrogen fuel cell systems. The key requirements for a fuel processor include rapid start-up, good dynamic-response to change in hydrogen demand, high fuel-conversion, small size and weight, stable performance for repeated start-up and shut-down cycles, maximum thermal integration, low cost and maintenance, high reliability and safety. In this respect, the development of a biogas steam reforming reactor, has been carried out at Institute CNR/ITAE, in order to be integrated into a proof-of-concept SOFC system, able to operate with biogas produced in an industrial waste water treatment unit. The design of a biogas reactor is the key aspect for the performance and efficiency of a hydrogen generator: weight and volume should be minimized and the heat management system optimized for different operating conditions.

Use of COMSOL Multiphysics®: Based upon the above considerations, a mathematical model, aimed at describing the performance of the reactor, has been developed. The mathematical simulations were achieved through the description of transport phenomena by Partial Differential Equations (PDEs), numerically solved through the Finite Element Methods (FEM), using the software package COMSOL Multiphysics® 4.2. The model covers all aspects of chemical kinetics and heat and mass transfer phenomena in the reactor. The model is able to couple fluid flow, heat and mass transport and chemical reactions occurring in the reactor. Momentum, energy, and mass balances have allowed to define the pressure, the linear velocity, the temperature and the products profile concentrations along the length of the reactor. COMSOL Multiphysics® was used to numerically solve the model equations and investigate the time evolution of the parameter characterizing the process (temperature, pressure, velocity, concentration).

Results: The aim of the model is to investigate the process performance of the reactor in order to enhance optimization and control of the steam reforming unit. Results showed that the overall performance of the reactor was strongly dependent on the reactor geometrical parameters (diameter and the length of the reactor) and on operating parameters (reaction temperature, H2O/CH4 ratio, CH4/CO2 ratio and gas hourly space velocity).

Conclusion: Simulation studies aimed at investigating the biogas steam reforming reaction have

been successfully performed by a two-dimensional mathematical model. A comprehensive investigation in order to explore component design, for understanding the performance limiting factors and identify possible means of process enhancement has been carried out. Parametric analysis was performed varying operating conditions such as inlet temperature and reaction parameters to study the effects on biogas steam reforming performance. Simulation results showed the strong dependence of the overall performance upon the reactor geometrical configuration. The model plays a key role in overcoming the issues of system design, by evaluating the temperature and concentration profiles along the length of the reactor.