Recent Developments of 3D Coupled Multiphysics SOFC Modelling at Forschungszentrum Jülich

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The Jülich SOFC modelling group has been performing 3D coupled multiphysics modelling of SOFCs, auxiliary components, as well as whole fuel cell systems since five years. Currently, emphasis has been given to the thermomechanical robust design and process optimisation of full-scale fuel cell stacks and whole fuel cell systems, including all auxiliary components. Particular attention is given to improve the understanding of the steady and transient processes, effecting the robustness and life-time duration of the components that directly influence the performance. Coupled CFD/FEM is used to mimic the thermofluid flow, electrochemical and chemical reactions, as well as thermo-mechanics.

Introduction

The Jülich SOFC modelling and simulation group has been built to aid in the development, design and optimisation of SOFC components, as well as to predict the processes of multiphysics nature, in 3D. The conducted research and development support and assist the overall SOFC development of Jülich, comprising the stack design and demonstration, manufacturing and characterization of different nature (1). Full commercialisation of the solid oxide fuel cell (SOFC) technology faces many technological challenges that impede the incorporation of the technology in the global energy sector. Problems such as leakage and hermetic sealing still endanger the durability and reliability of the fuel cell systems. Increasing the long-term and transient thermomechanical reliability of the interacting SOFC components and the associated fuel cell system demands a comprehensive understanding of the complex multiphysics, occurring within the system. The group is paying attention to investigate and improve the overall SOFC system design. Thereby, coupled 3D computational fluid dynamics (CFD) and computational solid mechanics (CSM) are employed for the solution of the complex problem. The models depict the true physical resolution of the components, as to mimic the complex behaviour as accurate as possible. Both material and geometrical non-linearity have been considered. Boundary conditions and model validation data are supplied from our component or full system tests. The supercomputers of Jülich are employed, where appropriate.
Current 3D Multiphysics Modelling Topics

All components and auxiliary parts within a solid oxide fuel cell system are assembled together and interact, thus contribute to the overall performance and robustness of the complex system. Understanding the Jülich integrated fuel cell system with its 20cm x20cm cell size, sheds light on the possible issues that may be present in large scale fuel cell systems, thus thorough investigations have been performed over the past time in various aspects (2-6). To understand and optimise the system in terms of process and thermomechanical durability, several focal points are set and pursued. A break through development has been the complete 3D computational fuel cell system model of the Jülich integrated fuel cell system. Single component modelling has been mainly used to assess the autonomous structural behaviour of components under thermomechanical load (7), and for design, performance optimisation purposes (8). A brief summary of some of the major activities have been elucidated.

Whole 3D Fuel Cell System Modelling

The design and allocation of each component plays a crucial role in the design of the entire multi-component system (9,10). The effort to increase the knowledge about the whole fuel cell system behaviour is limited to technological capabilities, as it is not possible to visualise and measure over time the local temperatures at every point within the SOFC system. Even to obtain this invaluable data provided at 700°C-1000°C entails an increased effort in experimental resources. Moreover, to gather information for a given system configuration, it is difficult to determine the optimal performance, proportioning of components and subsystems that interact and work together to yield the overall system characteristics (11). Recently, the detailed 3D multiphysics analysis of the whole system, simulated in fully resolution has been introduced (12). The heating process has been demonstrated and experimentally validated over 18 h time. The coupled thermofluid-thermomechanical behaviour could be fully visualised in 3D, as to determine the critical regions susceptible to high thermomechanically induced stress. Figure 1 demonstrates the system model cut from the mid region as to enable an inside view and the stress for a particular time instant.

Figure 1. The normal stress components in x-, y- and z-direction. The circled part of the full assembly is the bottom segment of the 36 layer fuel cell stack subjected to high thermomechanically induced stress.
The demonstrated results reveal that the manifold regions and the vicinity of the fuel cell adjacent to the upper baffle plates are subjected to higher stress. In practice, we measured significant leakage exact at the upper baffle manifold regions. It should be noted that the upper baffle is directly in contact with the fuel cell component that comprises at the outer sections and the manifold regions sealants, which are of brittle nature (11). The strain of the baffle plate leads to stress and strain in those regions. An important outcome is that the equivalent stress clearly reduced and became a more uniform distribution over time, supporting thermal results predicted by CFD that show that the initial stages of the heating-up process needs particular attention. The model, including all system components together with the sub-components is capable to perform coupled steady and transient CFD/FEM analyses for fuel cell dummy operation (without releasing heat from the fuel cell stack but accounting for chemically reacting species transport, reforming-shift, combustion, radiation in auxiliary components), as well as full operation stage of the system (with electrochemistry or heat sources mimicking the released fuel cell heat). The model accounts for the thermal, elastoplastic and time, rate dependent creep strain, as to completely describe the coupled thermofluid and thermomechanical behavior.

Fuel Cell Stack Modelling

The fuel cell stack component has been investigated in different modelling activities. The focus has been on the full scale 3D coupled thermofluid-thermomechanical modelling of short stacks. As the detailed operating stage analysis of full scale 36 layer SOFC stacks have been previously investigated in detail (13), major attention has been given to the thermomechanical behavior of six cell short stacks. In particular, the transient thermomechanical behavior has been analysed in detail during thermal cycling (14). Moreover, the effect of different operating environments and process conditions on the long-term thermomechanical behavior of fuel cells has been studied (15). The long

Figure 2. Comparison of the stress-strain behaviour of the metal components (15).
term creep strain behavior has been investigated in detail for over 1400 h, using a single unit of the stack, as to mimic better the single cell experimental measurements for validation purposes. Figure 2 depicts the comparison of the short stacks, operating in system (S) and furnace environment (F), respectively. The demonstration is for an analysis time of one hour.

Major outcomes have been that the lower stress during the furnace operation is dominated by the elastic strain of the steel material rather than the creep strain as the stiffer behaviour shows up in higher stress for the system operation. In this case the time the component is subjected load is not sufficient to relax the material, thus the creep contributes to additional strain. The manifold ports show higher creep strain at this location compared to the furnace operation (despite low), but still more stress compared to the furnace operation. Long term results of the single unit over 1400 h predicted the relaxation behavior and the associated decrease in stress of the interconnector, which on the other hand led to higher deformation and higher tensile stress within the glass components. Particularly, the outer long side of the stack has shown to be prone to high deformation of the steel, thus high stress in sealants, which is negative for the hermeticity of the stack. Post-mortem results of the stacks showed the regions prone to leakage and failure. The results show that stress on the component is decreasing with time and creep relaxation occurs. During the study, the long term structural behaviour could be predicted with the aid to estimate the service life-time of the fuel cells and to analyse the critical regions prone to failure due to creep strain.

**Outlook**

Current R&D performed using computational mechanics has been an invaluable tool as to visualise the processes and critical regions susceptible to failure, in 3D. The progress has reached a high-end standard as it has been possible to mimic a whole fuel cell system in 3D, thus showing that it is possible to use fully 3D modeling for system analysis rather than relying on conventional 1D analysis or black box models. Furthermore, the coupled multiphysics approach enabled to understand the effects on the long term behavior of fuel cell stacks that are considered within the design and optimisation stream in the development.

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**References**


