Hierarchical 3D Multiphysics Modelling in the Design and Optimisation of SOFC System Components

M. Peksen, Ro. Peters, L. Blum, D. Stolten

This document appeared in

Detlef Stolten, Thomas Grube (Eds.):
18th World Hydrogen Energy Conference 2010 - WHEC 2010
Parallel Sessions Book 1: Fuel Cell Basics / Fuel Infrastructures
Proceedings of the WHEC, May 16.-21. 2010, Essen
Schriften des Forschungszentrums Jülich / Energy & Environment, Vol. 78-1
Institute of Energy Research - Fuel Cells (IEF-3)
Forschungszentrum Jülich GmbH, Zentralbibliothek, Verlag, 2010
ISBN: 978-3-89336-651-4

Hierarchical 3D Multiphysics Modelling in the Design and Optimisation of SOFC System Components

M. Peksen, **Ro. Peters**, **L. Blum**, **D. Stolten**, Institute of Energy Research – IEF-3 Fuel Cells Research Centre Jülich GmbH, Jülich, D-52425, Germany

Abstract

This paper presents a novel bottom-up modelling approach to aid in the design and optimisation of the Research Centre Jülich type integrated module components. The approach is demonstrated by employing the air pre-heater component. A feasibility study substituting the real design with a simplified one is introduced. Analogue design simplifications are performed to the afterburner and pre-reformer component. The integrated module, including the simplified system components is simulated in 3D, considering the multiphysics that occur within each component. The predictions of the air pre-heater component are compared to the stand-alone air pre-heater simulation results. The results are in very good agreement. The approach is proven to be useful for the optimisation of the integrated module. Moreover, the results reveal that stand-alone component analyses are feasible, and can be used for the investigation of local processes, the development and construction of models, and the structural design optimisation of each individual component.

1 Introduction

The successful optimisation of the SOFC technology depends upon a thorough understanding of the whole system components and their interactions. The optimal proportioning and structural design of each component depends upon the process conditions it is subjected to. To peruse experimentally the effects of the design and operating parameters on each system component, or on the overall integrated module performance, is prohibitive; especially, at high temperatures. Computational modelling of individual Jülich type SOFC system components together with experimental validations has been elucidated in previous studies [1-3]. The use of computational modelling is an attempt to bring mathematical optimisation into the product development mainstream. However, the design of the individual components combined with the multiphysics, is very complicated. Moreover, 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. This implies that for a reliable and cost efficient optimisation, pursuing a systematic concept is indispensable. In a previous study [2], a systematic trio approach has been introduced to develop and employ an optimisation strategy for the design and optimisation of SOFC system components. Coupling this strategic concept with the design innovation is a challenging task.

This paper presents a novel hierarchically divided bottom-up modelling approach for the design and optimisation of the integrated SOFC module, developed and tested at the Research Centre Jülich. A combinatorial multiphysics analysis considering the fluid flow, heat transfer, chemically reacting species transport, and the thermo mechanics of the integrated module components, has been proposed.

2 Approach

The integrated SOFC module of the Research Centre Jülich is a complex system involving apart of the fuel cell, three more major components i.e., afterburner, air pre-heater and pre-reformer. Each component involves various processes contributing to the overall performance of the whole integrated module. To design and optimise the overall system performance, a hierarchically divided bottom-up approach is employed. Figure 1 depicts the general methodology.

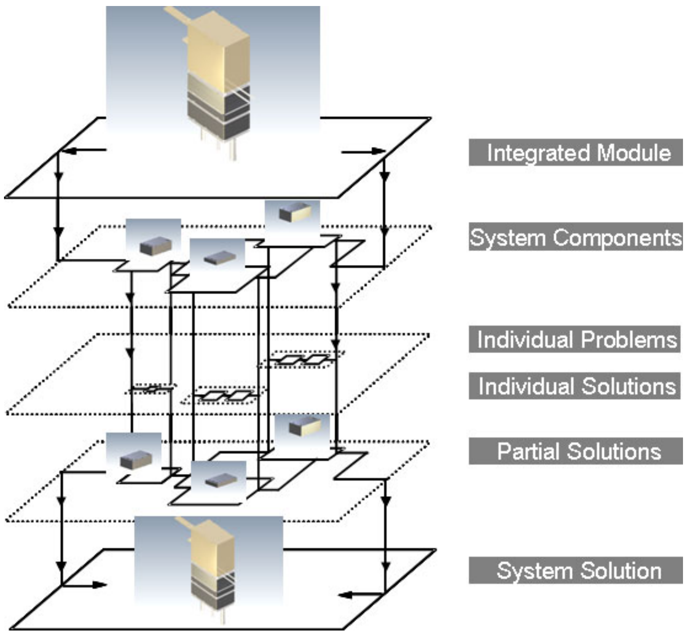
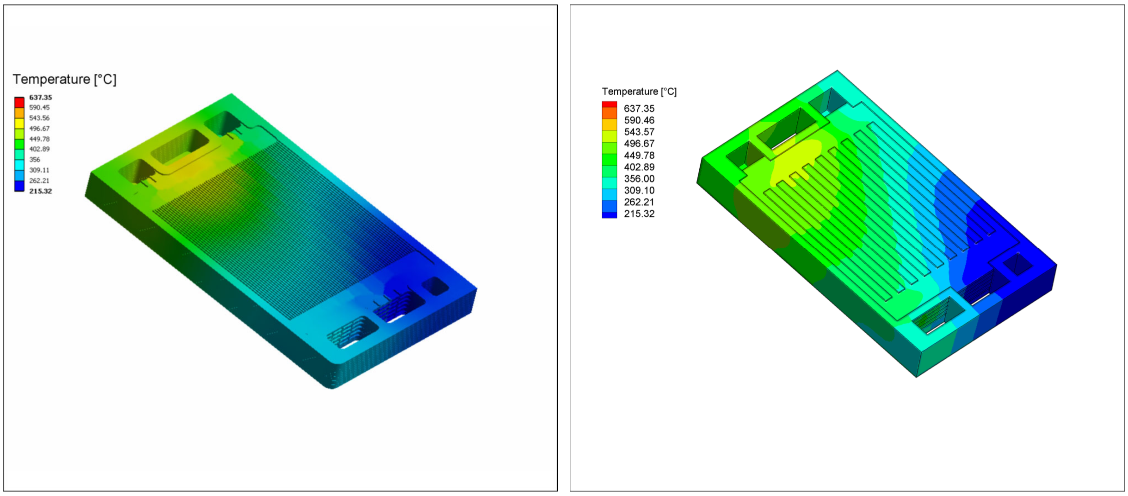


Figure 1: Schematic view of the employed bottom-up approach.

The full scale integrated module is virtually partitioned in stand-alone system components, each consisting of single unit assemblies stacked on top of each other. Each individual component comprises individual problems including additional sub components, different geometrical aspects and many different process conditions. This ensures the investigation of local processes, development and construction of models, and the structural design optimisation of each individual component. Moreover, this contributes much to a better understanding and prediction of each component's autonomous behaviour. The extrapolation of the obtained data will provide fundamental knowledge about the whole system behaviour. To verify the methodology, a feasibility study has been introduced and demonstrated on the air pre-heater component of the integrated module. The thermo fluid flow behaviour of the real air pre-heater design is compared to a simplified design. Analogue design simplifications are applied to the afterburner and the pre-reformer, mitigating the numerical difficulties associated with the geometrical and physical difficulties. In order to investigate the interaction of the air pre-heater with the peer components, the integrated module model is developed and simulated using the simplified component designs. The air pre-heater results predicted from the whole integrated module simulation are compared to the numerical predictions performed using the stand-alone air pre-heater component.

3 Results

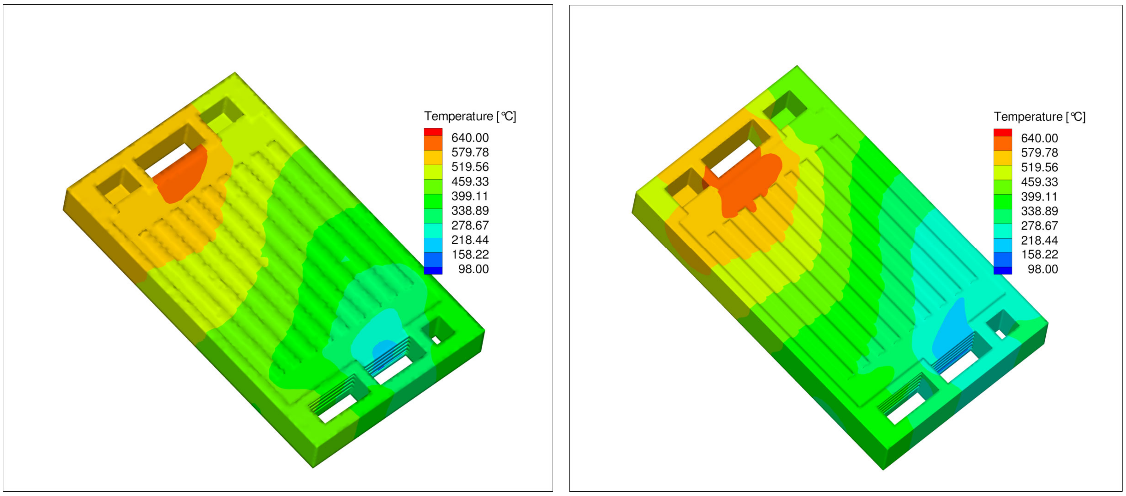
To test and verify the feasibility of the attempted approach, computational fluid dynamics is used to determine the thermo fluid flow behaviour of the real air pre-heater design and compare to the simplified design. The predicted results are illustrated in Figure 2.



(a) (b)

Figure 2: Temperature contour plot of the real pre-heater design (a) and simplified design (b)

The results show that the simplified design depicts the temperature profile of the real design reasonable. The cooler part of the pre-heater due to the reformer fuel is well captured. The distribution also reveals that a sufficient heat exchange could be achieved with a smaller design as well. Hence, substituting the real design with the simplified one is feasible. In order to understand the limits of investigating stand-alone components compared to an analysis performed with the whole system components, the simplified stand-alone air pre-heater is compared with the results of the pre-heater simulated considering all three system components i.e. afterburner, air pre-heater and the pre-reformer together. Figure 3 illustrates the comparison.



(a) (b)

Figure 3: Temperature contour plot comparison of the integrated module simulation (a) to the stand-alone component simulation (b).

The numerically predicted temperature profile obtained from the integrated module shows very good agreement with the stand-alone component. prediction. With negligible differences it can be stated that the demonstrated results of the stand-alone component are sufficient to obtain a better understanding about how each component performs within the integrated module and what impact the interaction of the components has on different physics of interest. The data provided enables to undertake an accurate design optimisation of each individual component.

4 Conclusions

A 3D bottom-up modelling approach has been proposed to design and optimise the Research Centre Jülich type integrated solid oxide fuel cell module. The feasibility to employ simplified component models has been tested and verified. The integrated module considering the whole system components i.e. afterburner, air pre-heater and the pre-reformer are considered in the model, including all physicochemical processes occurring within each component. Results predicted from the module simulation are compared to the stand-alone component simulation, being demonstrated using the air pre-heater component. Results are in very good agreement. The stand-alone component analyses enable a thorough investigation of each constituent of interest, providing detailed information about each component's autonomous behaviour. This ensures a reasonable component design optimisation Furthermore, it can be concluded that the stand-alone analyses yield to reasonable results, providing information about the component behaviour within the integrated module. The employed approach is proven to be an invaluable tool that can be used in local or global optimisations, in order to assist a rational new system design.

Acknowledgements

The technical staff of the SOFC Systems Technology Research Group, Research Centre Jülich is gratefully acknowledged.

References

[1] Peksen M., Peters Ro, Blum L, Stolten D., Numerical modelling and experimental validation of a planar type pre-reformer in SOFC technology, International Journal of Hydrogen Energy 34 (2009) 6425-6436.

[2] Peksen, M., Peters, Ro., Blum, L., Stolten, D., Component design in SOFC technology: 3D CFD modelling and experimental validation of a planar type pre-reformer, 6th Symposium on Fuel Cell Modelling and Experimental Validation, Bad Herrenalb/Karlsruhe, Germany, (2009).

[3] Peksen M., Peters Ro, Blum L, Stolten D., Component Design in SOFC Technology: 3D Computational Continuum Mechanics Modelling and Experimental Validation of a Planar Type Pre-heater, 7th Symposium on Fuel Cell Modeling & Experimental Validation, Morges (Lausanne), Switzerland, 2010.

[4] Peksen M., Peters Ro, Blum L, Stolten D., Design and Optimisation of SOFC System Components using a Trio Approach: Measurements, Design of Experiments, and 3D Computational Fluid Dynamics, Journal of The Electrochemical Society (ECS), Solid Oxide Fuel Cells 11 (SOFC-XI) Volume 25, Issue 2 pp. 1195-1200.