Cross-boundary Simulations of Fuel Cells

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Abstract. Simulation software systems play an important role in Automotive Fuel Cell System simulations. However, a considerable number of simulation system types are available on the market, which poses a dilemma for researchers. The question this review paper aims to answer is the following: What is the most effective way to choose the appropriate simulation system?

The paper (1) presents an inventory of typical issues that researchers seek to address and (2) discusses software that can help them find the solutions. When an issue can be addressed using several simulation systems, a comparison is made between them. When an issue is so complex that it cannot be addressed independently with any one of the available software, viable software combinations are proposed and examined. In such cases, the output of a software is used as the input for another, and the cross-boundary connections between them are addressed.

Finally, the paper presents a brief overview of modelling possibilities and a tabulated summary of the findings.

Introduction

Fuel Cells constitute a promising technology for the future, for example, because of their favourable environmental impact, efficiency, power density, and low noise level.

There are different types of Fuel Cells, but in the automotive sector the Polymer Electrolyte Fuel Cell (PEFC) is the most common. The PEFC generates electric current from electrochemical reactions between hydrogen and oxygen with the by-product of heat and water.

1 Fuel Cell System

A Fuel Cell System (FCS), as shown on Figure 1, has several components, which are defined in IEC 62282-1:2005 [1]. These components work together to produce electric and thermal power from the inputs of hydrogen, air, water, and the system also requires electric and thermal power.

The main components of a FCS are the Fuel cell stack; the air processing system, which contains a humidifier and a compressor; the fuel gas supply; and the thermal- and water management systems. Furthermore, there are several peripheral components such as pumps, valves, and electrical devices. The fuel and the air are not part of the FCS; they are fed into it.

The FCS and its parts raise many questions that researchers try to answer with the help of different types of simulation software systems. This paper aims to investigate which simulation software system are the most suitable for addressing the researchers' issues.

2 Fuel Cell Simulation Software Systems

There are several types of Fuel Cell simulation software systems available on the market, but only a few of them are used for scientific research.

This does not mean that the others do not work properly. Nevertheless, this paper only discusses those types of Fuel Cell simulation software systems that are preferred by the scientific community.

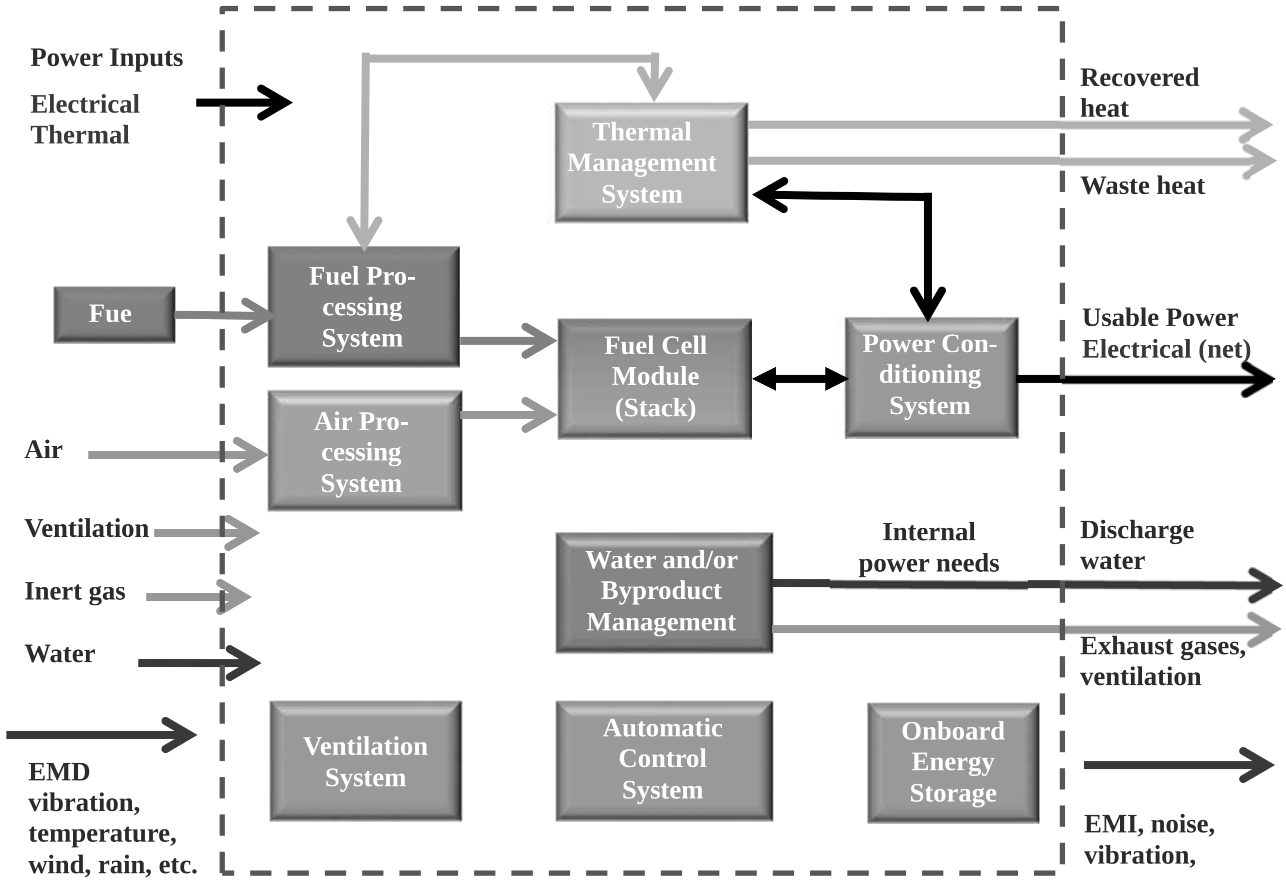

Figure 1. Fuel Cell System according to IEC 622882-1 [2]

These simulation software systems are:

- MATLAB®&Simulink®
- ANSYS Fluent
- AspenTech
- COMSOL Multiphysics

Each simulation software system has its own Fuel Cell specialised packages, which help making quick calculations.

Whereas these calculations may be sufficient sometimes, all of the packages have limitations that can only be solved by declaring equations and by setting up subsystems that are problem specific.

Cross-boundary Simulations are available between:

- MATLAB®&Simulink® and ANSYS Fluent by means of writing a journal file
- MATLAB®&Simulink® and COMSOL Multiphysics by means of MATLAB S-function and COMSOL Livelink
- MATLAB®&Simulink® and AspenTech Dynamics module by means of Control System Toolbox
- ANSYS Fluent and AspenTech by means of APECS [3]

ANSYS Fluent and COMSOL Multiphysics have been built for the same purpose; therefore, in their case there is no need for cross-boundary connection.

MATLAB®&Simulink® is mostly used for dynamic system simulations, ANSYS Fluent and COMSOL Multiphysics are suitable for Computational Fluid Dynamics, and AspenTech has been developed for chemical reactions and system optimizing.

3 Typical Questions

Some issues relate to an FCS as a whole whereas some others pertain to only a specific part of the system.

Issues
Stack operating conditions in different stack load points
Lower stack cathode pressure effect of FCS efficiency
Hydrogen consumption at different driving cycles
The effect of the compressor efficiency on the overall system efficiency
Stack idle operating conditions
Impact of the membrane resistance to the FCS peak efficiency
The impact of the compressor dynamic on the system dynamics

Table 1. Issues that can be addressed using MATLAB®&Simulink®[4]

Issues
Electrochemistry modelling
Current and mass conservation
Heat source problems
Liquid water formation and transport and their effects
Transient simulations
Leakage current

Table 2. Issues that can be addressed using ANSYS Fluent [5]

Issues
Fuel processing, hydrogen purification
Heat recovery, and water recovery
Steady-state material balances, heat integration
Dynamic analysis of heat-up, cool-down, power ramping
Safety analysis
Modeling of adsorption processes used to purify the fuel gas in the fuel conditioning section

Table 3. Issues that can be addressed using AspenTech [6]

Issues
Transport of charged and neutral species
Current conduction
Fluid flow, heat transfer, and the nature and driving forces of electrochemical reactions at planar and in porous electrodes
Design and optimization of the geometries and material choices of the system's electrodes, separators, membranes, electrolyte, current collectors and feeders with respect to performance, thermal management, and safety

Table 4. Issues that can be addressed using COMSOL Multiphysics [7]

4 Conclusion

In this paper, different kinds of simulation software systems have been reviewed. Tables 1-4 summarize the issues according to the simulation software systems with which they can be addressed.

None of the software can by itself provide the answers to all the questions, so for a complex analysis we need to use multiple software systems. Section 2 above presents the different feasible simulation software system combinations.

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