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1 Project execution

1.1 Introduction

The main objective of the project GenFC was to create a major contribution to the accelerated development of the fuel cell technology. Fuel cell technology is one of the key elements for the usage of sustainable energy sources. In the long term it enables us to produce electricity from hydrogen – which in turn can be obtained from biomass, wind power or solar power. In short and medium term fuel cells can be partly used to generate electricity from fossil fuels at high electrical efficiencies – thus, less CO$_2$ per kWh electricity is produced than by conventional power generating technologies.

The improvement of development process of fuel cells is approached by the project from two sides. Firstly, within the project several fuel cell models were developed which address current problems of the technology. Secondly, the modelling of fuel cells was brought one step further by combining all modelling expertise under one common umbrella, i.e. a structured framework. The idea of such a structured framework led to the development of the GenFC software – a modelling tool with database capability and defined interfaces that link individual fuel cell models and experimental data.

Fuel cell model development

The model development of the project addressed current problems in the area of:

- Improved description of the flow of reacting fluids in fuel cells and fuel cell stacks. For this approach the manufacturer of one of the most important computational fluid dynamics (CFD) software on the market – ANSYS/Fluent was working together with the specialized engineering company aixprocess.

- Hardware in the Loop (HiL) is a key technology in industrial product development. If one or more hardware components (in this case fuel cell devices) are not available at the beginning of the system integration process, they can be replaced in the laboratory by mathematical models that run on real time computers. The result are quick, cheap and safe development of system solutions by providing the possibility to investigate the performance of hardware components with realistic test rig based analyses. This task was performed by the Graz University of Technology, CD-Laboratory for Fuel Cell Systems.

- Fuel cell systems as part of a combined heat and power unit supplying heat and electricity to residential buildings have gained increasing attention. However, appropriate fuel cell system models for building simulation are not yet part of the standard distribution of building simulation software. The Swiss Federal Laboratories for Materials Testing
and Research (Empa) / Building Technologies Lab has extensive experience in the development of building and system simulation models for the software tool TRNSYS as well as in the application of simulation in research and in demanding planning tasks. The questions to be studied were details of the interaction of various components and long-term operation evaluation including energy efficiency, user comfort, and ecological and economical performance.

The GenFC software framework

The GenFC software is a modelling tool which was designed to be used in the field of fuel cell development and related simulations. The main feature is a database functionality which is combined with a test platform for models. It is designed to be easily extendable by programmers and easily usable by software users. It provides a standard format and interfaces for fuel cell models, simulation data and experimental results. The main objectives of the GenFC software are:

- to increase synergy effects in modelling,
- to share expert knowledge in the field of fuel cell related modelling with partners and
- to organize the in-house development process.

The GenFC software was developed in cooperation by software developers (partner REDHADA) and fuel cell modellers (partner FZ Jülich). The software is released as Open Source Project which makes it available to everybody without the need to purchase a licence. The present status of the GenFC software is a beta-release, which makes it suitable to be used at research centres and universities, where new features can be added by programmers and the software can be developed further. The end of the project GenFC marks the starting point of the ripening process of the GenFC software – it is intended to be used and modified according to each university or companies needs.

The Forschungszentrum Jülich (as example) has a great interest in continuing the work on the GenFC software. It was already shown at the 8th European Fuel Cell Forum in Lucerne (Switzerland) how the GenFC software shall be integrated in the R&D activities of Forschungszentrum Jülich. After the end of the project the development of the GenFC software will continue in a series of diploma theses, the first thesis started already in October 2008. In this way the generic architecture of the GenFC software is exploited to add new features as the need for them arises.
### 1.2 List of Participants

<table>
<thead>
<tr>
<th>Name</th>
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<tbody>
<tr>
<td>Forschungszentrum Jülich GmbH&lt;sup&gt;a&lt;/sup&gt;</td>
<td>Germany</td>
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<tr>
<td>Fluent Deutschland GmbH&lt;sup&gt;b&lt;/sup&gt;</td>
<td>Germany</td>
</tr>
<tr>
<td>Swiss Federal Laboratories for Materials Testing and Research (EMPA)</td>
<td>Switzerland</td>
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<tr>
<td>Graz University of Technology, CD-Laboratory for Fuel Cell Systems</td>
<td>Austria</td>
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<tr>
<td>aixprocess PartG Verfahrens- und Strömungstechnik, Ingenieure Dr. Weng und Partner</td>
<td>Germany</td>
</tr>
<tr>
<td>REDHADA SL</td>
<td>Spain</td>
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<sup>a</sup>Coordinator

<sup>b</sup>Fluent Deutschland GmbH is a subsidiary of ANSYS Inc. - after the end of the project, Fluent Deutschland GmbH has been renamed to ANSYS Germany GmbH.
1.3 Modelling of transport processes

Fuel cells which operate at temperatures below 100°C are so called low temperature fuel cells. There are several different types which all have in common that inside these fuel cells a complex interplay of gaseous components (air and hydrogen) and liquid components (water) can be observed. This leads to several specific multiphase phenomena, which complicate the modelling of these devices.

1.3.1 The basic principle of the low temperature fuel cell

The basic principle of a low temperature fuel cell is explained in short at the example of the direct methanol fuel cell (DMFC). Methanol is used as fuel in this type of fuel cell, a mixture of methanol and water is fed to the DMFC anode compartment (left side of figure 1). In the middle of the fuel cell there is a polymer electrolyte membrane which separates anode and cathode side of the fuel cell. The methanol is converted to carbon dioxide, protons and electrons at the anode side. The carbon dioxide is transported towards the anode compartment, as the polymer electrolyte membrane is nearly impermeable to gases. The protons are transported through the polymer electrolyte membrane to the cathode side. There, the protons and electrons reduce oxygen (from air) to form water. The water leaves the cathode catalyst layer towards the cathode compartment. Concurrent to the proton diffusion through the membrane the transportation of water from the anode side to the cathode side takes place. This water flux through the membrane is called electro osmotic drag and it is of non-negligible size (i.e. it is a problem).

![Figure 1: Principle of the direct methanol fuel cell (DMFC)](image)

In summary, all these electrochemical reactions combined with the occurring drag flow lead to a specific amount of water entering the cathode channel. The amount of water depends on the operating point of the fuel cell. If too much water is produced on the right side of figure 1, the air
channel is blocked and the fuel cell does not operate properly. To recognize the right amount of water (which is influenced by transport processes as well as electrochemical processes), special attention has to be paid to the modelling of this multiphase phenomena.

1.3.2 CFD simulations in general

Computational Fluid Dynamics (CFD) provides a numerical model of things that flow and can thus be applied to simulate fuel cells or fuel cell stacks. Fuel cell simulations typically involve a three dimensional description of the fuel cell where geometric features are well resolved in the underlying mesh to correctly capture the fluid, heat, and electric current flow.

ANSYS Inc offers modules for its commercial CFD code FLUENT that allow to simulate Proton Exchange Membrane Fuel Cells (PEMFC) and Solid Oxide Fuel Cells (SOFC). This involves the calculation of fluid flow, heat transfer, electrochemical reactions, and other effects (e.g. the PEMFC model includes models for membrane water transport and liquid water formation).

Fluent\(^1\) provided an interface to make the fuel cell module for PEMFC and SOFC of the commercial CFD code FLUENT work together with the GenFC software. This way it is straightforward to use the commercial fuel cell software from Fluent together with GenFC.

1.3.3 1D-in-3D: Low dimensional approximation of gas channels

Fuel cells are energy converters that use fluid fuels in combination with air (or pure oxygen) in order to produce energy. Inside typical low temperature fuel cells these fluid components follow a ‘jungle’ of small and curved channels (see figure 2). This makes the numerical simulation of such fuel cells computationally very challenging.

The 1D-in-3D approach rests upon the fact that the pipe flow in a gas channel is in itself typically laminar and that spatial features in the flow are typically not of interest. It is therefore tempting to simulate this channel flow as one dimensional (1D), depending only on the length coordinate along the channel. Meshing the other parts of the fuel cell in the traditional three-dimensional (3D) fashion, the 1D gas channels simply penetrate this 3D mesh and may exchange mass, species, and heat with it, which is why this approach has been termed 1D-in-3D.

\(^{1}\)Fluent Deutschland GmbH is a subsidiary of ANSYS Inc.
Figure 2: Gas channel jungle of a fuel cell stack. Cathode inlet manifold with connected cathode gas channels and respective anode gas channels below. The insert shows a top view demonstrating the intersections seen in projection through the stack. Geometry courtesy of FZ Jülich, mesh by Fluent.

The 1D-in-3D approach has been implemented into the commercial CFD code FLUENT making as much use as possible of the available solver infrastructure. Work was required mostly on the following topics:

- internal data structures for 1D mesh cells
- 1D mesh generation
- automatic generation of terminal connections that link the ends of a 1D channel to three dimensional (3D) volumes
- automatic generation of lateral connections that link a 1D channel laterally to a surrounding 3D volume
- numerics of terminal and lateral connections
- numerics of non-straight 1D channel flow, like around a bent
- numerics of 1D gradients for field variables in the 1D channel
- Correlations for lateral exchange of mass, momentum, heat, and species between 1D channels and a 3D volume. All of these transport mechanisms are required to describe the action of a gas channel in a fuel cell.
The design decision to implement the 1D-in-3D functionality into the core FLUENT solver allows for a unique feature: The transport across terminal and lateral connections can be treated fully implicitly, i.e., there is only one linear system solved for any field variable regardless whether a particular value belongs to a 3D or a 1D mesh cell. This yields a dramatic increase in numerical stability and robustness compared to a purely explicit handling.

In a typical 1D description of fluid flow, the flow velocity will be described by a single scalar for the velocity’s sign and magnitude while its direction is determined by the direction of the 1D region. In 1D-in-3D this is different. Because the 1D mesh cells are handled by the same solver as the 3D mesh cells, the equations solved are the same. This implies that three partial differential equations (PDE) are solved for the three components of the velocity field also in the 1D mesh zones. This makes it necessary to have additional measures to guarantee that the flow in the 1D mesh zones stays aligned to the direction of the 1D mesh. The flow may be misaligned to the 1D direction, if either it enters a 1D mesh zone at an angle different than the 1D direction or if within a 1D mesh zone there is a bend. To achieve the alignment of the flow, a robust numerical algorithm is in place to provide the necessary force perpendicular to the 1D direction. Figure 3 demonstrates the effect. Since the 1D mesh zones are necessarily unresolved in the lateral direction, the effective transport in this direction must be modeled by correlations. Meaningful defaults for pipe flow are available as well as a programming interface to apply arbitrary user specified correlations.

![Figure 3: Velocity vectors of the flow field in a 1D helical mesh. The velocity vectors are tangential to the circular shape of the helix.](image)

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1.3.4 Experiments with a transparent fuel cell

A transparent fuel cell has been developed at the Forschungszentrum Jülich to get a qualitative impression of the formation and movement of the liquid phase in the product channel of the fuel cell. The experimental set up can be seen in figure 4. A mixture of water and methanol flows through the anode channel of the fuel cell and air flows through the cathode channel. The experiments are performed for common operating points of fuel cells.

![Figure 4: Set up of the transparent low temperature fuel cell test device](image)

Figure 5 shows the liquid water in the product channel of the fuel cell at a characteristic working point. It can be seen that some channels seem to be free of droplets while the walls of other channels are covered with droplets of different sizes. The diameter of these droplets is lower than 0.1 mm. These small droplets stick more or less motionless to the walls. The drag force, imposed on the droplets by the gas flow, is not high enough to overcome the adhesion forces. Beside the small droplets a much lower number of bigger drops with a mean diameter greater than 0.5 mm could be observed. These drops flow down the channel walls and on their way down to the outlet of the channel they grow by collecting all the smaller droplets on their way. The experimental results give a qualitative impression of the effects taking place in the fuel cell channels. The applied fuel cell device is not appropriate to measure the pressure drop in a channel as a function of the amount of liquid water or the gas flow rate respectively. Moreover no additional information concerning the droplet formation in fuel cell channels could be extracted from literature. Hence detailed simulation studies have been made to determine the effects of droplets on the course of the pressure drop.
1.3.5 CFD simulation of drop movement

According to the observations made at the fuel cell experiments (figure 5) numerical simulations have been carried out to analyse the movement of a single drop and a row of drops through the cathode channel of the fuel cell. The formation of droplets on the membrane surface depends on to many uncertain parameters, which are not fully determined yet. Due to the lack of information, the simulations have been carried out neglecting the initial formation of droplets. It is assumed that the water entering the channel instantaneously forms a droplet that grows depending on the amount of water flowing through the membrane. Simulations have been carried out to calculate the pressure drop of the air for a single drop moving through the cathode channel of the fuel cell. The calculations have been performed for different droplet diameters.

These 2D studies have been made for a vertical channel with 1 mm in height, 1.5 mm in width and 22 mm in length. The inlet gas velocity is 0.5 m/s. At the beginning of the simulation the channel is filled with 10 droplets. The diameter of the first droplet is 0.5 mm, the diameter of the other droplets is 0.3 mm. The channel is divided into 22 equidistant segments. In each segment the concentration of the liquid phase is calculated. Figure 6 shows several snapshots of moving droplets in the channel. At the beginning the gravitational force and the gas flow accelerate the droplets downwards to the outlet of the channel. The acceleration of the bigger droplet is slower than the acceleration of the smaller droplets, but in the end the bigger droplet moves faster through the channel than the smaller droplets. The higher gas velocity between the droplet surface and the channel wall causes a higher drag force on the droplets. Once the bigger droplet has speeded up, the distance between the big droplet and the small droplets reduces. When the big droplet reaches the nearest small droplet they coagulate to form an even bigger droplet. This in turn leads to an acceleration of the bigger droplet, which then collects more and more smaller droplets. At one point the size of the droplet exceeds the cross section of the channel and the droplet blocks the channel.
Figure 7 shows the corresponding pressure drop and liquid phase concentration in four selected segments of the channel. It can be seen that as long as the concentration of the liquid phase is lower than 0.6 the pressure drop is made up of the sum of the pressure drops caused by each droplet. When the liquid phase concentration exceeds this value the pressure drop in the channel also increases. Now the droplet starts to block the channel. This in turn results in a higher pressure drop. The imposed inlet velocity and the blockage of the channel lead to some numerical instability, which are the reasons for the oscillating pressure drop in figure 7.
1.3.6 CFD study of the outlet geometry of the cathode channel

The developed multiphase 1D model for PEFC and DMFC is subject to restrictions concerning the outlet geometry of the cathode (air) channel. Additional 2D simulation studies have been carried out to analyse the influence of the channel outlet geometry on the movement of the drops. The geometry of the channel outlet has been changed from a sharp-edged outlet to an outlet with rounded edges. The simulations have been performed for different radii of the rounded edges. Figure 8 shows the movement of some droplets flowing through the channel towards the sharp-edged outlet. The channel height is 1 mm. The numbering $t_1$ to $t_{10}$ in figure 8 simply refers to the different time steps of the pictures. The simulation starts at $t_1$, three drops are patched into the channel with an initial velocity of 0 m/s. The gravitational force acts in downward direction. The inlet pressure is set to 1 Pa. During the simulation experiments it could be seen that the droplets start moving. Due to the different diameters of the drops the acceleration of the drops differs slightly. The smallest drop is the one near the sharp edged outlet of the air channel; naturally this drop reaches the outlet first. But instead of flowing around the corner, the drop bounces back from the corner and flows upward the channel. The gravitational force as well as the air flow in the channel forces the droplet to change its flow direction again towards the outlet of the channel. The process of bouncing back and moving towards the sharp edge repeats until the drop comes to rest at the sharp edge. The middle drop also moves towards the outlet of the channel and coagulates with the smallest drop sticking at the sharp edge (fig. 8: $t_3$). But even the formed bigger drop is not able to flow around the corner of the outlet. When the third drop reaches the outlet it coagulates with the other drop (fig. 8: $t_5$). The formed new drop is big enough to block the complete channel (fig. 8: $t_6$). With an inlet pressure of 1 Pa it is not possible to break the blockage of the air channel. The high surface tension of the drops prevents them from flowing around the sharp edge of the channel outlet. This has also been observed in some
experiments. To break this blockage a significant increase of the inlet pressure is necessary. With an inlet pressure of 100 Pa it is possible to blow the blocking drop out of the air channel (fig. 8: t₈ to t₁₀). In case of a real fuel cell the blockage of the channel persists and the gas flow will be redistributed on the remaining open channels. The process of redistributing the airflow on the open channels will continue until the overall pressure drop is high enough to break the blockage.

Figure 8: Movement of single droplets through the air channel towards a sharp edged outlet. t₁ to t₇: Pressure driven flow with an inlet pressure of 1 Pa; t₈ to t₁₀ pressure driven flow with an inlet pressure of 100 Pa

An optimisation of the outlet geometry should be performed to enable a continuous outflow of drops out of the channel. It could be seen in figure 9 that if the radius of the rounded edges is to small the high surface tension prevents the drop from flowing around the corner (fig. 9, a). On the right hand side of figure 9 an optimised outlet geometry is shown. The shape of the optimised outlet is an ellipsoid with a radius bigger than the channel height. The 2D simulation studies showed that the design of the air channel outlet strongly affects the outflow of the droplets. The developed 1D multiphase model can only be used when the continuous outflow of the droplets is guaranteed. The accumulation of drops at the end of the channel is not comprised in the model.
1.3.7 Virtual test rig

The aim of the virtual test rig is to determine the drag force coefficient depending on the average air velocity and the diameter of the drop. The test environment is a two dimensional image of the fuel cell air channel (fig. 10). The channel is 1 mm in height and 20 mm in length. A drop of defined size is placed near the lower wall in the centre of the channel. The gravitational force is set to zero. The air enters the channel on the left hand side with a defined velocity. The gas flow pushes the droplet towards the outlet of the test channel. To prevent the droplet from getting blown out of the channel a force field is applied onto the droplet that acts against the flow direction of the air. A control system has been implemented that centres the drop in the middle of the test channel by modifying the force field. Once the drop reaches a stable position in the middle of the channel, the drag force is found for a drop with a defined diameter and a defined relative velocity between the drop and the gas flow.

Performing the above described experiment for different inlet velocities of the air and different drop diameters lead to the diagram in figure 11. It shows the drag force coefficient versus the
Reynolds number $Re$:

$$Re = \frac{\rho_a d_h |v_{air} - v|}{\eta_a}$$

(1)

with the hydraulic diameter $d_h$ of the free cross section in the channel above the drop, the relative velocity $|v_{air} - v|$ between the liquid and the gas phase, the air density $\rho_a$ and the air viscosity $\eta_a$.

The correlation between the drag force coefficient and the Reynolds number has been approximated by the equation $\xi = a \cdot Re^b$ with the coefficients $a = 2.5e5$ and $b = -0.78$.

### 1.3.8 The 1D multiphase model

The 1D multiphase model has been adapted to the 1D-in-3D concept which was developed by the partner ANSYS/Fluent. Figure 12 shows the discretised air channel. In the present case, the channel is divided into small cells of 1 mm edge length. This means that the free cross section of the channel is covered by only one cell. The eulerian approach has been chosen to calculate the two-phase flow in the channel. For each phase the momentum and the continuity equations are solved. In these equations the inertia force, the gravitational force and the interphase exchange force are included. So far the CFD software of ANSYS/FLUENT does not allow for the calculation of the adhesion force, which is obviously caused by the lack of experimental data concerning the hysteresis of the contact angle. For the time being the adhesion force is neglected in the 1D multiphase model. Concerning the interphase exchange force the CFD software of ANSYS/FLUENT only delivers models for swarms of droplets flowing through a continuous medium. In case of the air channel of a fuel cell only single drops flow through the air, hence a C-routine has been written to calculate the interphase exchange force.
The required drag force coefficient and its correlation with the Reynolds number have been determined in the virtual test rig (fig. 10). In a first approach the diameter of the droplets in each cell is dependent on the local liquid fraction. It is assumed that the density of drops is 1 drop per cubic millimetre. Condensation and water flow through the membrane should be implemented as source terms for the liquid phase in each cell.

Figure 12: 1D discretisation of the air channel
1.3.9 Large scale fuel cell simulations

The geometry of a realistic PEFC from Forschungszentrum Jülich will serve as the basis for a comparison of the new 1D-in-3D concept against the conventional 3D approach. Fluent generated a traditional 3D mesh using the geometry provided by Forschungszentrum Jülich, which took several weeks by an experienced CFD-engineer. The mesh of a single cell is depicted in figure 13. This was used to create a stack with 5 PEMFCs including endplates (for an impression of the channel geometry, see figure 2 on page 7). The resulting mesh has about 9.3 Mio mesh cells.

The simulations were carried out in cooperation of Fluent and Forschungszentrum Jülich on the supercomputer IBM p6 575 (JUMP). These have been the largest fuel cell simulations performed so far to the knowledge of the project’s participants. A glimpse of the results has been collected in figure 14.
1.3.10 1D-in-3D Demonstration

Fluent conducted first fuel cell simulations with the new 1D-in-3D capability and compared them to fully resolved 3D simulations. To this end a single straight channel PEMFC was used with the following dimensions: 5 cm length, 6.4 mm width, and 7 mm height. The geometry with fully resolved gas channels and the respective 1D-in-3D geometry are shown in figure 15. In the 1D-in-3D geometry, the 1D gas channels are located at the centers of the true gas channels and are displayed as thin lines. The mesh of the original gas channels has been merged to the respective bipolar plates.
Figure 15: Straight channel PEM fuel cell simulation (top = cathode, bottom = anode)

Figure 16 shows velocity and temperature for the case using the 1D-in-3D approach. In these figures, the box in the lower part depicts the anode bipolar plate, and the upper plane represents the top boundary of the cathode bipolar plate. The 1D gas channels are shown as lines. These results demonstrate that the principal 1D-in-3D functionality is working as intended.

Figure 16: Velocity and temperature for the 1D-in-3D approach

The left part of figure 16 shows velocity vectors in the 1D gas channels which are coloured by velocity in m/s. The inlets are at the rear, the outlets at the front. The right part of figure 16 shows the temperature in °C in the PEMFC: in gas channels (lines) / in the interface between cathode electrode and membrane / and in planes vertical to the channels. The colouring of the lines representing the anode and cathode gas channels shows that the temperature increases in the channels.
1.4 Hardware in the loop

Fuel cell models can not only be applied in theoretical analyses, but also in test rig based component and system development. If one or more hardware components of a fuel cell system (e.g. a hydrocarbon reformer or an offgas afterburner) are to be tested in real-life conditions, hardware-in-the-loop (HiL) often is the technology of choice. In HiL, production or prototype hardware components of a system – where the term 'system' is referring e.g. to a combined heat and power fuel cell system for domestic cogeneration or a fuel cell propulsion system for vehicle applications – are interfaced to simulated components in order to be able to investigate the combined operation of the overall system. Thus, operation of the components can not only be investigated individually but in combination with the whole system. The interdependence between the components can then be investigated and easily identified. The actual hardware components can be operated as if the whole system is present, although only selected components are actually available and operated in the safe environment of a laboratory test rig. Utilizing this functionality, fuel cell component and system developers are able to apply real time approved fuel cell models available within the GenFC model database in HiL applications in a user-friendly, flexible and efficient way.

1.4.1 GenFC hardware-in-the-loop application

Based on the commercial real time target hardware solution from National Instruments Corporation, a general interface concept was designed and implemented in the software LabVIEW. Two main functions are available for HiL applications: a real time core and a visualization terminal prototype function. The purpose of the real time core is to run fuel cell models under real time conditions, and to provide the interfaces to read in sensor signals and to write control signals to actuators. Error handling and communication interfaces are also readily implemented to provide a maximum level of safety in real time operation. The overall layout of the GenFC HiL concept is shown in figure 17. The dashed line indicates the functionality provided by the real time core, and therefore includes the whole processing of signals between the sensor and the control levels plus the associated functionality. The real time core prototype function is readily provided by the GenFC software; application-specific adaptations can be easily made in dedicated user functions. All the user has to provide in order to be able to fully use the GenFC HiL solution is a LabVIEW installation and a computer/controller capable of real time operation.
The complete GenFC HiL solution consists of four different elements:

- the FC model, available as C-written DLL and human-readable model parameter text file within the GenFC model database,
- the real time core as real time specific LabVIEW implementation
- the visualization terminal for remote access and finally
- the real time target hardware, a specialized computer hardware where the software can be executed in real time conditions.

The visualization terminal is provided by the GenFC software. Communication interfaces from and to the application terminal are readily installed to enable remote communication between the test rig and a remotely located desktop PC (e.g. a desktop PC located in the office building communicating with the real time target hardware located in the workshops near the test rig).

A screenshot of the application terminal main screen is shown in figure 18. The application terminal is intended for providing remote access to the real time core function and provides a compressed overview of real time FC model status and operation as well as signals coming from sensors or generated for actuators, respectively. A control sidebar is included to provide short access to key information and control tools. A number of different control and visualization
panels are included on the right hand side of the terminal to provide detailed information about setup, model configuration and operation.

Figure 18: Screenshot of the PEMFC/HiL application terminal main screen
1.5 Simulation of building energy supply systems

One possible application of fuel cell systems are cogeneration devices used in buildings to provide heat for space heating and domestic hot water at the one hand side and electric power on the other hand side. Figure 19 shows a prototype of a residential SOFC-cogeneration device. Figure 20 shows schematically how such a fuel cell cogeneration system device is integrated in the energy supply system of a building and connected to the electricity grid.

![Figure 19: Residential 1 kW SOFC-cogeneration device](image)

The integration of such a fuel cell co-generation device in a building energy supply (as shown in figure 20) gives raise to the following challenges.

- The control strategy of the complete device (not only the fuel cell itself) must be in aligned to the overall building control.
- What is the overall performance of an energy supply system using a fuel cell co-generation?
- What is the optimal size of such a device for a certain building?

To answer these challenges building and system simulations are needed. There are many simulation programs available which include models of the building structure and usual components of building energy supply systems. The GenFC software provides now tools and models used for the simulation of energy supply systems with fuel cell co-generation devices, which either are not standard components of most simulation programs or have to be set up with a big effort within the simulation program. The following tools and models can be exported either as model or project objects from the GenFC database.
Load Generator Tool to produce stochastic electrical and domestic hot water load profile data

EE-Module Post processing tool for economic and ecological analysis

FC-system model Dynamic model of a fuel cell co-generation device

Building and System Model Assembly of the whole building and system simulation model

1.5.1 Load generator

The electric and hot water load generator tool produces typical, random time series of domestic hot water and non-HVAC (heating, ventilating, and air conditioning) electrical loads for a whole simulation period, e.g. one year. These load profiles can then be used as input data for dynamic building and system simulation. They can be generated for a single apartment / single family house, multiple apartments / multi family house or even a cluster of multi family houses. Methodologically, stochastic single usages are generated and superposed. This statistical approach is event-based. That means, loads are defined as events which are characterized by a start time, a duration and a certain power or intensity (see figure 21). The probability that a single event occurs is defined with a relative distribution within a day and a frequency distribution per day, both set per weekday. Additionally, a frequency distribution for the power and the duration of the event can be set. These distribution characteristics are defined for certain load categories of electric and hot water demands of different household types. The categories are
not predefined but can be chosen as needed and can be specified at any level of granularity.

Figure 21: On / off events and resulting electrical profile for one load category

The electric demand may be split into: cooking, baking / lighting / washing / entertainment (stereo, TV, PC, ...) / other (hair drying, lawn mowing, vacuum cleaning, ironing, ...).

The hot water demand may be split into: short load (washing hands, etc.) / medium load (dish-washer, etc.) / bath / shower.

The household type is: single / working couple / family / elderly couple.

The superposition of the load categories, and, if multifamily houses are considered, households results in the total load profile. The time resolution of the resulting profile data can be set at any value. Occupancy is considered by a list of weekly and non-recurring absences, which are stochastically varied and simultaneously valid for the electric and the hot water load series. Thus, a relation between the electric and hot water series is ensured.

The tool is implemented in MATLAB using its statistical and graphical possibilities. Figure 22 shows the front end of the tool. The model has been compiled into an executable which runs without requiring a MATLAB license. Excel sheets are used for data input and for result summary output. The resulting load profiles are stored in text files which then can be read by any simulation software.
1.5.2 Ecological economic module

The ecological economic module (short: EE-module) adds ecological and economic analysis to building and system simulation. Ecological and economic indicators are used for an assessment of the system under consideration within a life cycle perspective. The EE-module has been implemented as an Excel sheet, which can be used for post processing of results from dynamic building and system simulation. The period of analysis is the same for ecological and economic analysis. Because of the seasonal characteristics of building energy supply, the length of the period is fixed to one year. Figure 23 shows the principal structure of systems analyzed with the EE-module. Heat and possibly electricity is generated onsite, stored and distributed. Electricity and energy for heating and domestic hot water is delivered to satisfy requirements for comfort and services. Electricity may in addition be purchased from the grid or sold to the grid. The electricity supplied from the grid is produced by the specific mix of power stations in the grid. Depending on operation strategy and operation requirements, there may occur heat or electricity dumps. The onsite generation is associated with direct emissions and / or waste. System boundaries are in any case identical for both ecological and economic analysis. The economic analysis is based on the total annual costs caused by the annuity of the investment capital, electricity and fuel demand and additional costs. The analysis is performed with real
Figure 23: Principal structure of systems intended to be analysed with the ecological / economic module. DHW = domestic hot water

costs, i.e. costs and interest rate are inflation-adjusted. This allows using constant annual costs for energy demand and operation.
Electricity costs may either be calculated within the EE-module or supplied as input. In the latter case the costs can be calculated within the building system simulation. This is necessary if structured tariffs such as time dependent prices and combined energy usage and capacity demand charges are applied. Within the EE-module the annual electricity costs are calculated with the electricity price and the annual net electricity delivered from grid, which is the difference between the electricity demand and the locally generated electricity. If more electricity is generated than demanded then the resulting electricity costs are negative, i.e. the result is rather a revenue then a cost.
The annual fuel costs are calculated with the fuel price and the fuel demand. The additional annual costs comprise the costs for operating, servicing, insurance and tax. They are a user defined project specific input. The ecological analyses rely exclusively on the electricity in- and output and the fuel input calculated with the dynamic simulation for a one year period. The in- and outputs induced by fabrication, installation and disposal of the components are ignored. Non renewable primary energy demand and CO₂ equivalent emissions are used as decisive ecological indicators.
1.5.3 FC system model

In the frame of IEA annex 42, a FC-cogeneration device model was developed and implemented in several different building and system simulation programs.² The FC system model describes the residential SOFC-cogeneration device shown in Figure 19. Measured data of an actual prototype have been used to calibrate the model parameters. The device has a nominal rating of 1 kW electric and 2.5 kW thermal power output. The assumed performance characteristics are given in figure 24 as electrical and thermal efficiencies – in relation to the lower heating value (LHV of natural gas fuel) – as function of the actual power input of the fuel (LHV) and for three water return flow temperatures (at inlet to SOFC unit). The integrated auxiliary heater has a nominal rating of 9.5 kW thermal power output. The generated electricity is directly used in the house or else delivered back into the electric grid. The electric grid is also used to cover peak demand.

After the calibration the electrical efficiency has suppositionally been improved and as a result the model adapts the thermal efficiency accordingly. This assumed improvement of the electrical efficiency is based on industry expectations to be realistically achieved within the next couple of years. The efficiency specified is somewhat smaller than the electrical efficiency of actual

large industrial SOFC systems. It seems reasonable for small residential SOFC-cogeneration
devices considering that parasitic energy was also accounted for. The characteristics shown in
figure 24 have been produced using the model with the parameters adjusted as described. A
modulation range from 480 W to 1 kW electrical power output is assumed. The change of the
modulation from one time step to the next is not restricted. This implies a maximum power
output change of at least 0.6 W/s which is a value probably too high for current prototypes.

Different building energy demand levels were considered by defining two building sizes and
three energy standard levels. A single-family house (SFH) and a multi-family house (MFH)
with 4 dwellings were considered and for each of the two building types, three thermal insu-
lation levels and respective heating, ventilating, and air conditioning systems (termed energy
levels) were specified.

- Building according to the average Swiss residential building stock
- Building complying with Swiss building code (standard SIA 380/1 2001)
- Low-energy building according to the Passive House standard

The geometric layout of the MFH is basically a multiplication of the SFH type building geo-
metry (see figure 25). All dwellings have the same internal floor area of 188.8 m².

The thermal properties of the building envelope (insulation and glazing), and the building equip-
ment and appliances are adapted to the different energy levels of the buildings. The heat dis-
tribution and ventilation systems assumed for the individual building types are described in
table 1.
<table>
<thead>
<tr>
<th>Energy demand level</th>
<th>Building type</th>
<th>Swiss stock</th>
<th>Swiss code</th>
<th>Passive House</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>SFH</td>
<td>MFH</td>
<td>SFH</td>
<td>MFH</td>
</tr>
<tr>
<td>Space heat demand</td>
<td>516</td>
<td>518</td>
<td>172</td>
<td>154</td>
</tr>
<tr>
<td>Electricity demand</td>
<td>51</td>
<td>68</td>
<td>54</td>
<td>67</td>
</tr>
</tbody>
</table>

Heat distribution and ventilation system for individual building types

<table>
<thead>
<tr>
<th>Heat distribution</th>
<th>Ventilation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hydronic convectors (27% radiative)</td>
<td>Natural ventilation by window airing with 2.1 m³/(h m²)</td>
</tr>
<tr>
<td>Hydronic floor heating, embedded in concrete slab</td>
<td>Natural ventilation by window airing with 0.7 m³/(h m²)</td>
</tr>
<tr>
<td>Hydronic floor heating, embedded in concrete slab</td>
<td>Balanced ventilation with heat recovery (68%); 120 m³/h per dwelling; 0.1 h⁻¹ infiltration in zones with external doors</td>
</tr>
</tbody>
</table>
1.6 GenFC software framework

1.6.1 Introduction

The overall goal of the GenFC software is to provide a generic modelling tool to fuel cell and fuel cell systems developers making fuel cell modelling expert knowledge available to all of them. The fuel cell and fuel cell systems developers can then use this tool to improve and accelerate fuel cell development and to contribute to a future success of the fuel cell technology. It is believed that from the fuel cell (hardware) developer’s point of view, a fuel cell modelling environment is desirable which can be used for simulation tasks exactly catering to the demand of the application engineer. The user of such a modelling environment expects to be able to chose a model out of a set of different types of fuel cells. Each type of fuel cell can be available in different implementations and each implementation is suitable for a particular application. The GenFC software provides a database with graphical front end to store all models and related information. This includes documentation, input parameters and results of simulations. The software is released as Open Source Project which makes it available to everybody without the need to purchase a licence. Not included in the free release is the contents of the database. The scope of this project is not to create a single huge database. Each research group or company can create it’s own database with models and data according to their needs. This is one generic aspect of GenFC.

Furthermore, GenFC is a generic modelling framework. It provides defined interfaces for models which enables the user to couple models to applications (or other models). The framework has a modular and extensible architecture. New applications and functionalities can be added easily. GenFC is not restricted to special commercial simulation software. It is designed to keep the modelling data from different software applications together. Thus, the GenFC software can assist to organize the in-house development process and exchange of information (modelling or experimental data) with external partners.

1.6.2 The software

The GenFC software will be available for download in January 2009 from www.genfc.org. The present status of the GenFC software is a beta-release, which makes it suitable to be used at research centres and universities, where new features can be added by programmers and the software can be developed further. The end of the project GenFC marks the starting point of the ripening process of the GenFC software – it is intended to be used and modified according to each university or companies needs.
The GenFC software consist mainly of a Back End server and a graphical user Front End. The function of the Front End is:

- to give the user a Graphical user Interface to request information from the Back End, store and retrieve data and
- to provide a simple test environment for stand alone models (some graphical output, ...) which can easily be extended by programmers to incorporate new features

The function of the Back End Server is:

- provide requested data to the correspondent requesting Front End client,
- permanently store coherent and organized Modeling data in a database,
- support concurrent and secure access: several users can access Back End modelling data simultaneously.

The GenFC software is multi-user and platform independent (both Front and Back End). The Back End and Front End are designed to follow a client / server architecture (figure 26). It is recommended to restrict the software to local installations, since no specific security measures are incorporated – which would be required for an open web access.

Figure 26: Front End / Back End configuration of the GenFC software
As the database management system, PostgreSQL has been chosen. PostgreSQL is an object-relational database management system, released under a BSD-style license.

**Object Storage**

The GenFC software will provide fuel cell models and related data to the users. This data is organized in 3 different data objects: model, parameter and project.

**Model** The model object contains the fuel cell (or any other) model as binary or source code. Additionally, several keywords are applied in order to generate a hierarchy for browsing and exploring.

**Parameter** The parameter object contains a complete set of input variables for a specific model. These variables can be manipulated by the user. Additionally the information of the corresponding model (in the database) is contained.

**Project** The project object contains user data. This can be results of a simulation or any other third party software files (e.g. MATLAB, FLUENT, TRNSYS, SIMULINK, ...). Additionally, the information about the applied model and parameter objects are stored.

The user is able to search and browse the contents of the database through a single interface (Front End). The GenFC Back End has the ability of dealing with simultaneous concurrent data browsing coming from different users. For browsing the database some kind of order or hierarchy is required. This functionality is provided by keywords and their values. The user will see only data objects owned by himself / herself and public data objects. An example for the result of a database search for models is shown in figure 28.
1.6.3 Generic interface

The integration of GenFC models to system simulation software can be separated into two programming interfaces. From the bottom view, each model is connected via the general application interface to a module interface coupling. While the general application interface is almost independent from the system simulation software, the application specific interface is dedicated to a particular third party software (e.g. MATLAB, FLUENT, TRNSYS, SIMULINK, ...). It handles all data structures and the access from and to them which are specific to the external system simulation software. In figure 29 an example for the interface coupling for systems simulation is shown.

Figure 28: Results of a database search for a model
The programming interface specified as generic interface for fuel cell stack models in figure 29 is already in use in the EC project LargeSOFC (project no. 019739 of FP6) for component models developed at Forschungszentrum Jülich. In the EC project LargeSOFC, Jülich is developing simulation models for three components which are coupled to system simulation software. In that project, two different software packages for system simulation are used. With the generic interface for fuel cell models, the coupling software of component models to system simulation had to be developed once for each of the two software packages. After that, every component model which provides the generic interface for fuel cell models can easily be compiled for use in one of the supported software packages for system simulation.

Figure 29: Programming interfaces for fuel cell models
2 Dissemination and use

2.1 The GenFC software

The GenFC software is a modelling tool which was designed to be used in the field of fuel cell development and related simulations. The main feature is a database functionality which is combined with a test platform for models. The software is released as Open Source Project which makes it available to everybody without the need to purchase a licence. A user manual and tutorials were created that explain the basic functionalities of the software. This will enable a novice user to use GenFC. In order to demonstrate the capabilities of the software, a model\(^3\) from the literature was implemented, which simulates the characteristic current-voltage behavior of a high temperature polymerelectrolyte fuel cell. It is executable from within the GenFC software, i. e. no additional software is required. A screenshot of the model’s results is shown in figure 30.

\[\text{Figure 30: Screenshot of the HT-PEFC model}\]

\(^3\)The model describes the ”working range” of a HT-PEFC, i. e. the range where the relation between current and voltage is nearly linear.
The end of the project GenFC marks the starting point of the ripening process of the GenFC software – it is intended to be used and modified according to each university or companies needs. As a major fuel cell developer in Europe, the Forschungszentrum Jülich is interested in using the GenFC software as an end user to improve the turn-around cycles of the fuel cell hardware development.

In order to distribute the GenFC software it is important to show the benefit for possible customers. Therefore, a semi-commercial dissemination of the GenFC software is planned, the partner aixprocess will be responsible for that. One possible way to show the benefit of the product is to create something like a basis version, which is for free. This basis version comprises the whole functionality of the database and a package of simplified models for each level of model refinement (sub-cell, cell, stack and system models). This enables the customer to use the database and its special functionalities for his own developments (models, system models, database, structuring, analysing data etc.). The provided simplified models show the customer additional functionalities of the product. The simplifications of the models are necessary to prevent problems with copyrighted models. An extension of this basis version is possible. We can offer the customer the possibility to enlarge their model portfolio by buying additional models. In figure 31 a possible structure is shown, which enables the dissemination of the GenFC software together with additional models.

![Dissemination concept of GenFC](image-url)
The partner aixprocess can act as the distributor of the software and will be responsible for the maintenance of the website which is shown in figure 32. The support for the basis software is minimal. The partner aixprocess will keep the contact to the customers of the basis version. If a customer needs a special fuel cell or system model that is available in the model portfolio of the GenFC package, aixprocess will sell it to him. If the model is not available, aixprocess will try to figure out the possible partners, who are able to develop and implement the model. Then the new model is sold, depending on the price it is sold to one customer exclusively or it is taken into the pool of models.

This structure enables the distribution of different fuel cell models in one package and it offers the possibility of other model developers to sell their models via this platform. In this structure the partner REDHADA acts as the specialist for databases. This concept fulfils two conditions. On one hand it is free for everybody to improve or support the model development and to exchange the models with other partners. On the other hand it offers the possibility to sell and buy special models, via the distributor of course.
The FZJ is one of the leading research institutions in Germany with about 4200 employees. Energy technology is one of the main research topics with an involvement of approx. 350 person-years. Protection of the environment and natural resources, economy and safety are among the prime research goals. Over the past decade the FZJ has been involved in several national programmes on SOFC co-operating with industries like Siemens and Barker|Bennett|EconTech as well as in several European projects co-operating with research institutes (ECN Petten, NL, Royal Rohdeius, DK) and industries. Recently the FZJ was involved in two EU projects dealing with SOFC plant development (ProCor) and the improvement of the long term stability of cell components (SureSGFD). Currently the FZJ is involved in one IP (RealSGFC) concerned with finding solutions for the persisting ageing problems of SOFCs. Besides a long history of over decade in SOFC research, there is also an LTFC research activity primarily concerned with DMFC research but also with PEFC research.

Modelling has always played an important role in Fuel Cell development at the FZJ as there is extensive experience with model development and validation. The FZJ has introduced the first three dimensional computer code for the transient simulation of SOFC stacks operating with internal reforming of methane. The model equations used in that computer code for describing the electrochemical reactions and the internal reforming process are still being used today by SOFC modelers all over the world and have established a standard in SOFC modelling. However, LTFC modelling is a new activity at the FZJ and there is not much experience yet in this area. Since GenFC is a generic integrated modelling tool, it must have an LTFC modelling capability.

www.fz-juelich.de

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Figure 32: Future website of http://www.genfc.org
2.2 Product: CFD: 1D-in-3D coupling (partner: FLUENT)

The 1D-in-3D functionality provides the knowledge of how to implicitly couple the solution of partial differential equations on connected 1-dimensional and 3-dimensional regions. It is planned that this knowledge will be available as part of a computational fluid dynamics (CFD) software. Direct exploitation will be in extending the CFD software to simulate fuel cell stacks with many 1-dimensional regions.

2.3 Product: Hardware in the loop (HiL) model (partner: CDL)

HiL is an industrial key technology commonly applied in the development of hardware solutions for a wide range of applications e.g. in the automotive industry, in aerospace applications, or in automation and process engineering. The basic approach pursued in applying HiL technology is to combine the flexibility of a mathematical simulation with the development process of a hardware component. Fuel cell models with HiL capability are primarily required by:

**Automotive industry** for development of fuel cell power trains or auxiliary power units (APUs).

**Process engineering** for development of combined heat and power systems (distributed power generation).

**Fuel cell systems component development** for development and testing of system components (e.g. fuel processors, heat exchangers and power electronics).

The GenFC HiL concept, developed by CDL, introduces a convenient way of providing fuel cell models to application-oriented scientists and engineers working in pre-commercial and commercial test rig applications. The concept is currently based on commercially available third party software and hardware solutions. It might be interesting to develop a fully integrated package consisting of a custom-written software solution for test rig operations and data logging procedures - maybe directly implemented with a future version of the GenFC software - and a custom hardware solution assembled from commercially available hardware components but tailored to the specific type of application served with the GenFC software. This might be a possible way of commercially exploiting the GenFC HiL concept if users of the GenFC software provide the feedback that they would be interested in such a HiL package. This will be particularly relevant if fuel cell technology manages to become more attractive for commercial applications in terms of availability and costs. Fuel cell models will most likely not be exploitable in terms of selling them or licensing their use, but only if there are integrated in a package such as GenFC.
2.4 Product: Tools for building simulation (partner: EMPA)

The following two software tools can be used together with any building simulation software. They will be part of the basis version of the GenFC software distribution.

Load generator

The model provides load profiles for household electricity and domestic hot water demand to residential building simulation. It has been implemented in Matlab using Matlab’s statistical and graphical possibilities. The tool has been compiled into an executable which runs without the Matlab software. Excel sheets are available to prepare the input for the load generator and the resulting load profiles are stored in text files which then are inputs to any building simulation software.

Ecological economic module

This model calculates investment and running costs, CO₂ emissions and primary energy use of cogeneration or heating systems. It is developed mainly to analyse FC based cogeneration systems, but it will not be limited to such systems. The economic and ecological feasibility of the system under consideration can be assessed and compared to the performance of other competing systems. The tool has been implemented as an Excel sheet, which can be used for post processing of results from dynamic building and system simulation.

2.5 Product: TRNSYS models (partner: EMPA)

Fuel cell cogenerarion device model

In the frame of IEA Annex 42 a model for a fuel cell cogeneration device has been developed and implemented in several building and system simulation software tools. The implementation of this model in the building simulation software TRNSYS has been further developed in the frame of the GenFC project.

- Model parameters can now be input in a more user friendly way with a separate input file.
- Model outputs have been added in order to allow for a whole system energy balance check.
- A graphical representation of the model (proforma file) for the graphical user interface of TRNSYS has been added.
- The Model is now available with two different Interfaces: a) With the TRNSYS specific interface to plugin in the TRNSYS user library and b) with a generic FC-System interface to use the model from any other higher system modelling software tool.
Building and system simulation model

The residential building and system simulation model is designed for the use with fuel cell and other cogeneration device models. It is implemented in the building and system simulation program TRNSYS. The model includes the building structure, the energy supply system and the energy management and control system. A set of six different residential buildings (three different energy demand levels and two different sizes) is provided with the model. The building and system simulation model has been set up with Simulation Studio, the graphical user interface of TRNSYS.

The models and tools developed by EMPA within the GenFC project will all be available for the public as they will be included in the database of the publicly available version of the GenFC software. EMPA will use them in further research projects, e.g. in the ongoing EU FP6 project POLYSMART where the performance of fuel cell cogeneration systems in combination with thermally driven absorption cooling devices will be modeled and evaluated.