DESIGN, SIMULATION AND EVALUATION OF DOMESTIC MICRO-CHP UNITS

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ABSTRACT

The limitation of the greenhouse effect and global warming will be the most important and challenging task of the next decades. One contribution being discussed is the introduction of new technologies in the domain of domestic energy supply for homes. Cogeneration units, also known as micro combined heat and power units (micro-CHP), claim to a significant overall-increase in efficiency compared to conventional heating installations. However, as of now only a few micro-CHP technologies have reached the product level resulting in limited installed units. As a result, experience and results from actual installations are not widely available. We have developed simulation tools that allow us to calculate precisely the costs, availability, efficiency and CO_2-savings of various micro-CHP technologies, including fuel cell micro-CHP units. The results can then be compared with one another, as well as with data from conventional heating installations, making it possible to identify the benefits and shortcomings of each technology. Further more, the results of simulations can also be used to identify areas with high potential for optimization and to guide future development.

INTRODUCTION

The issue of environmental protection continues to gain in importance. While few pollution problems, such as NO_2-based stratospheric ozone depletion seem to have become less dramatic (EPA, 2003) others, such as carbon dioxide emissions and the related greenhouse effect (Alley et al., 2007 / EPA, 2006) demand urgent action.

One widely discussed way to contribute to environmental protection and pollution reduction is to introduce new technologies in the domain of domestic energy supply for homes. Cogeneration units, also known as micro combined heat and power units (micro-CHP), claim to be able to increase overall efficiency and to create significant CO_2 savings compared to conventional heating installations (Harrison, 2004 / Frei-Hardt, 2005). Typical micro-CHP heating units are based on Stirling engines, Rankine cycles, internal combustion engines or fuel cells (FCs). In the UK, micro-CHP had been identified as a key element of the Government's energy strategy (DTI, 2003).

While some micro-CHP technologies have reached the readiness for marketing (Harrison, 2004), the overall number of installed units is still quite low in many countries (DTI, 2005 / Pfeifer, 2005). There are therefore limited experience and results from actual installations available.

Computer-aided simulations provide an alternative approach to investigating and analyzing the system characteristics of micro-CHPs. While simulations on the chemical and physical levels are necessary for the design and construction of single components or elements of components, modeling on the thermodynamic and system levels is required in order to model, analyze and optimize an entire unit.

In this paper, we present simulation tools that have been developed to accomplish multiple types of system simulations, with the focus on fuel cell cogeneration units. In the second section, “Thermodynamic Modeling of fuel cell micro-CHP Units”, we discuss techniques for modeling a complete unit as a composition of multiple components. Principles of physical and thermodynamic conservation, media composition and representation, equilibrium chemistry, thermodynamic states and properties, phase changes and balancing are addressed. In the third section, “System Simulations”, we present methods for performing rapid, yet precise simulations of entire systems, e.g. a house including its heating installation. Such simulations make it possible to calculate costs, availability, overall efficiency and CO_2-savings, as well as to compare various heating system technologies, including micro-CHP units versus conventional heating installations. In section four, “Results and Discussion”, we present a selection of results we have generated. Working from such results, areas with high potentials for optimization can be easily identified and guide future development.

THERMODYNAMIC MODELING OF FUEL CELL MICRO-CHP UNITS

There are at present many simulation tools available for chemical and physical modeling of hydraulic and thermodynamic components. Some typical examples include FEMLAB, Fluent, Modelica, Dymola and ASPEN. Such tools allow highly detailed modeling of chemical and physical processes. However, modeling

an entire unit, composed of dozens of parts and components, sharply increases the effort involved in implementation as well as the simulation time.

Since it is necessary to conduct thermodynamic modeling on the system level in order to model, analyze and optimize an entire unit precisely, other simulation tools were needed. An additional requirement was preferably to design and evaluate the complete control application for such micro-CHPs in the same development environment as the simulation. The decision was made to use MATLAB/Simulink, which allows the user to conduct modeling, simulation and controller design on the same platform.

One drawback of Simulink is that thermodynamic modeling is barely supported. Therefore, the thermodynamic Simulink library FClib was developed, providing simulation blocks for

- representation and balancing of flow masses,
- thermodynamic and conservative calculations,
- equilibrium and reaction chemistry,
- typical components and assemblies, and
- adjustment of species used.

Modules for thermodynamic simulations

The library we developed provides a collection of modules such as pumps, fans, compressors, valves, splitters, mixers, heat exchangers, humidifiers and humidity exchangers, dryers, burners, chemical reactors, and last but not least fuel cells and inverters, as Fig. 2.1 shows. These modules are used to easily set up a complete micro-CHP unit simply by selecting and connecting the required modules.

Media flows are represented by objects, encapsulating the following media properties:

- molar flow
- temperature
- pressure
- enthalpy flow
- entropy flow
- free Gibbs enthalpy flow
- heat capacity flow
- composition of flow
- media gaseous fractions
- media molar fractions

All component modules as well as the flow objects are based on thermodynamic property and state calculations, which are discussed in the following section.

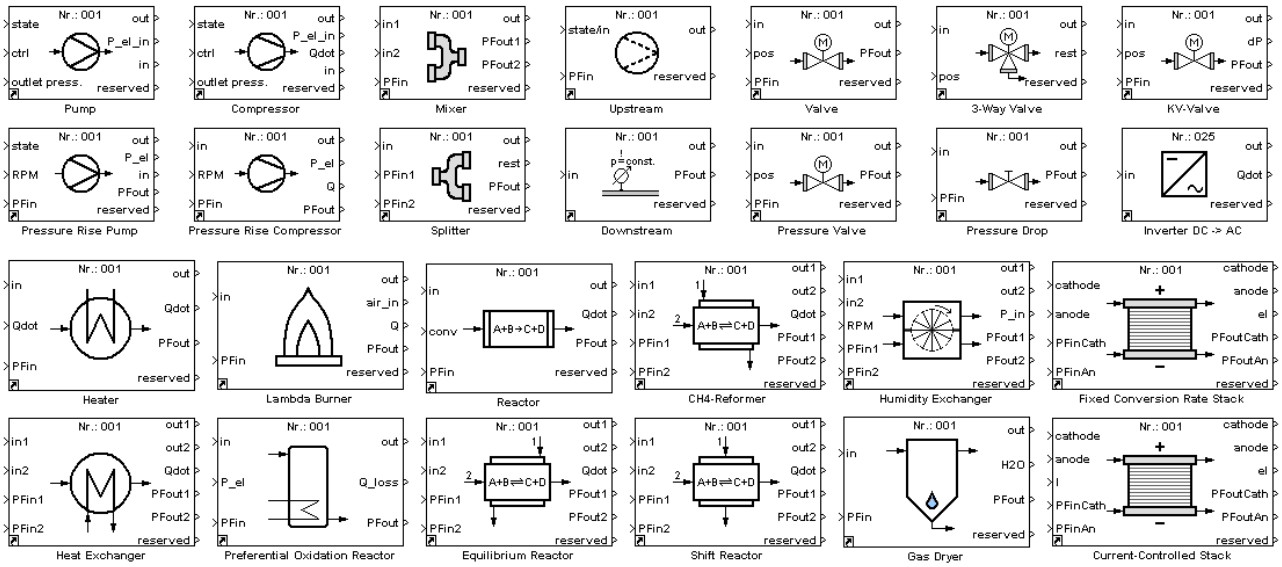


Fig. 2.1: Extraction of modules of the simulation library

Thermodynamic fundamentals

Thermodynamic states and transformations are basically represented by their enthalpy, entropy, free Gibbs enthalpy and heat capacity. These are calculated based on the JANAF-thermo physical tables, using the NASA polynomial representation (Gordon, 1971). Eq. (2.1) to (2.4) give the calculations for gaseous phases at temperatures between 200 K and 6000 K.

$$H_m/(RT) = A + \frac{B\cdot T}{2} + \frac{C\cdot T^2}{3} + \frac{D\cdot T^3}{4} + \frac{E\cdot T^4}{5} + \frac{F}{T} \tag{2.1}$$

$$S_m / R = A\cdot \ln(T) + B\cdot T + \frac{C\cdot T^2}{2} + \frac{D\cdot T^3}{3} + \frac{E\cdot T^4}{4} + G \tag{2.2}$$

$$G_m = H_m - S_m \cdot T \tag{2.3}$$

$$C_{pm} / R = A + B\cdot T + C\cdot T^2 + D\cdot T^3 + E\cdot T^4 \tag{2.4}$$

For liquid phases the heat capacity C_p is typically assumed to be constant. In this case enthalpy, entropy and free Gibbs enthalpy are given by Eq. (2.5) to (2.7).

$$H_m = H_{m,298[K]} + C_p (T - 298K) \tag{2.5}$$

$$S_m = S_{m,298[K]} + C_p \ln\frac{T}{298K} \tag{2.6}$$

$$G_m = H_m - S_m \cdot T \tag{2.7}$$

Chemical reactions, e.g. within a reactor block such as a CH4-Reformer or a Shift Reactor, are described by general reaction equations according to Eq. (2.10).

$$v_A A + v_B B \Leftrightarrow v_C C + v_D D \tag{2.10}$$

The corresponding chemical equilibrium relation is given by

$$\ln\left[\frac{a_C^{v_C}\cdot a_D^{v_D}}{a_A^{v_A}\cdot a_B^{v_B}}\right] = -\frac{\Delta G^0}{\overline{R}T}\ , \tag{2.11}$$

calculating the mole fractions of the outgoing flows (Sonntag, 2003), with

$$a_i = \frac{y_i P_i}{P_i^0} \tag{2.12}$$

being the activity coefficients for the given components´ mole fractions y_i.

ΔG^0 is given for constant temperatures by

$$\Delta G^0 = \Delta H^0 - T\Delta S^0\ . \tag{2.13}$$

The chemical equilibrium equation, Eq. (2.11), is solved using Eq. (2.13). In this way, we obtain the mole fractions of the equilibrium mixture.

Simulations

Complete micro-CHP units are modeled by selecting and interconnecting modules, where each module represents a component of the real process. This makes it possible to set up the simulation models in a way similar to the process flow-charts.

Different connections and piping can be evaluated by simply changing the signal connections. The same holds true for analyzing different process technologies, e.g. a preferential oxidation (PROX) compared to a methanizing reactor: by exchanging the corresponding modules, any process technology can be

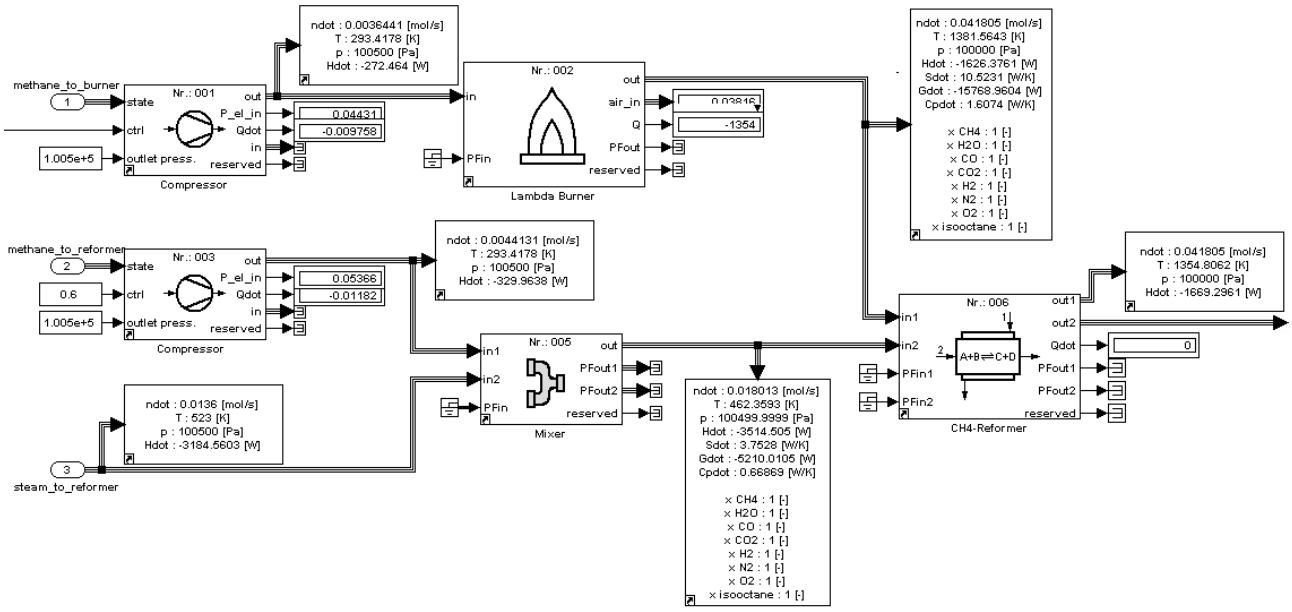


Fig. 2.2: Model (extraction) of the gas production of a fuel cell micro-CHP unit

evaluated as well as optimized in conjunction with the whole unit. Fig. 2.2 shows an example of the gas production of a fuel cell micro-CHP unit.

Since the simulation environment Simulink makes it possible to design and evaluate complete control applications, it is possible to introduce software development techniques such as model based design and Rapid Control Prototyping (RCP) (Mlynski, 2004 / Turoni, 2005) and include them into the design of the entire micro-CHP. Controller applications are mandatory for micro-CHP and will be discussed in the section “Results and Discussion”.

SYSTEM SIMULATIONS

As discussed in the previous section, detailed thermodynamic simulations are performed in order to design and evaluate heating installations. However, simulations on a system level are performed to gather information about the system as a whole, e.g. a house including its heating installation. Simulation results are typically used to

- inspect the system’s behavior and performance,
- calculate costs, availability, efficiency, CO_2-savings, etc.,
- compare different heating installations,
- identify areas with high optimization potential and
- guide future development.

Requirements for system simulations

To accomplish the goals mentioned above, several requirements must be met. Upon development of the simulation tools discussed in this paper, a major focus has been set for these requirements.

First of all, consumption data are required that represent the house’s energy consumption used in the simulation. Such consumption data comprise the thermal energy for heating and hot water supply as well as water and electrical energy consumption. There are two different well established approaches for collecting consumption data. One is to develop a model of the house and to simulate the household consumption depending on the season, the outside temperature, the insulation, the number of people residing in the house, their habits, and so on. An alternative approach is to measure real data in the field and enter it into the simulation. Though the second approach requires measuring large sets of data, these data are completely realistic, since they are based on actual measurements.

The simulation discussed in this paper utilizes the second approach as shown in Fig. 3.1: all of the consumption data measured in the field are used as input data for the simulation. The heating installation is simulated to deliver energy in accordance with these input data. The simulation results are the operating

power of the installation at each simulation step, the gas consumption, the buffer filling degree, the net balance, the costs and CO_2 emission, among other factors.

The second requirement on system simulations is that they possess the ability to perform simulations over extended periods. Simulating just a day or a week typically does not give enough information on the system's performance, nor on its overall costs, efficiency, etc. Setting up four different weeks, representing the four seasons of the year, implies to many erroneousness when projecting the results to a complete year. Simulating longer periods, i.e. months up to several years, is thus inevitable.

This requirement, simulating over months or years, raise another necessity: besides being absolutely precise, simulations must also be fast. If one were to set up a model of a new heating installation and then conduct a simulation of one year, it would not matter whether that simulation took an hour or half a day. Yet as we will show, simulations of heating installations include dozens of parameters. These parameters must then be altered upon evaluation and optimization. Since different combinations of parameter values have different effects, multiple simulation runs have to be conducted in order to evaluate the system completely. As a result, simulations not only have to be very precise, but extremely fast, too.

Last but not least, tools for optimization, e.g. automatic determination of optimized parameters, are necessary. Such tools include the definition of and minimization of cost functions or heuristic search algorithms. In combination with the previously mentioned rapid simulation, such tools make it possible to perform a comprehensive analysis of an entire system within a few hours.

Simulation set-ups

To simulate a system, the modeled heating installations are set up in the system simulation environment. The simulation environment includes the modeling of additional components such as hot water tanks and peak load heaters (PLH), which are used in particular in fuel cell micro-CHPs (FC-CHP). Fig. 3.2 shows the block diagram of the FC-CHP discussed in this paper.

For each system, around 50 parameters must be set in order to adapt the simulation to an existing heating installation:

- Hot water tank
  Volume, surrounding temperature, heat loss due to radiation and convection, temperature set point, etc.
- Fuel cell
  Minimum/maximum thermal and electrical power, efficiency, startup and shut down times, blocking times, controller parameterization, etc.
- Peak load heater
  Minimum/maximum thermal power, efficiency, startup and shut down times, blocking times, controller parameterization, etc.

Simulations are performed with variable step size solvers to achieve two goals: maximum simulation resolution, especially in areas with dynamic transitions, and maximum simulation speed. The simulation environment discussed in this paper allows simulations that are typically 150,000 times faster than real time, making it possible to simulate a complete annual cycle with a resolution of one minute in approximately four minutes on a conventional 2.8 GHz Pentium 4 processor.

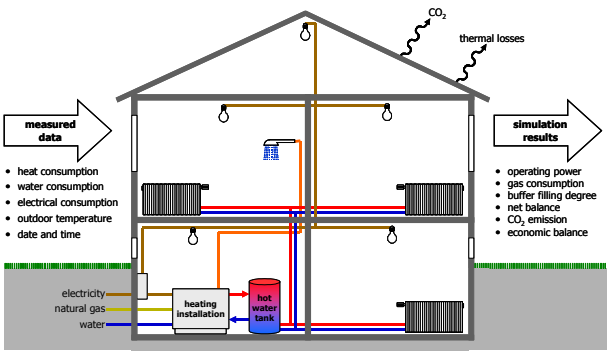


Fig 3.1: Inputs and outputs of system simulations

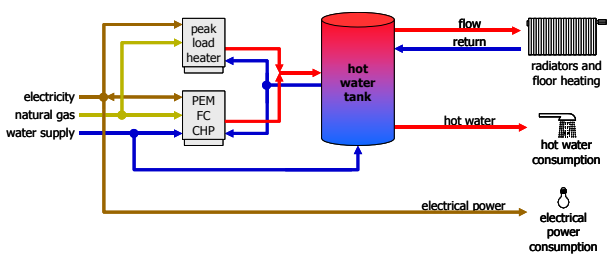


Fig 3.2: Block diagram of a FC-CHP unit

RESULTS AND DISCUSSION

Several FC-CHP units have been modeled and simulated. After designing these models, we conducted an analysis of them. Fig. 4.1 shows the isobar vaporizations of a media flow with phase changes at different pressures (T-s diagram).

A focus was set on proton exchange membrane (PEM) fuel cells. These fuel cells can be driven with pure hydrogen only. Therefore, PEM FC-CHP have a gas production on board, reforming natural gas to hydrogen (Pukrushpan, 2004). The first production step is to reform methane (CH_4) within the so-called steam reformer reactor. According to Eq. (2.10), the two reactions that take place in the reactor are given by Eq. (4.1) and (4.2).

$$CH_4 + H_2O \Leftrightarrow 3H_2 + CO \tag{4.1}$$

$$CO + H_2O \Leftrightarrow CO_2 + H_2 \tag{4.2}$$

The corresponding chemical equilibrium relations are given by Eq. (4.3) and (4.4).

$$\ln\left[\frac{\left(y_{H_2} p_{H_2}\right)^3 \cdot \left(y_{CO} p_{CO}\right)}{\left(y_{CH_4} p_{CH_4}\right) \cdot \left(y_{H_2O} p_{H_2O}\right) \cdot p_0^2}\right] = -\frac{\Delta G^0}{\overline{R}T} \tag{4.3}$$

$$\ln\left[\frac{\left(y_{CO_2} p_{CO_2}\right) \cdot \left(y_{H_2} p_{H_2}\right)}{\left(y_{CO} p_{CO}\right) \cdot \left(y_{H_2O} p_{H_2O}\right)}\right] = -\frac{\Delta G^0}{\overline{R}T} \tag{4.4}$$

The first reaction, according to Eq. (4.1), is strongly endothermic. The heat energy required is supplied by a lambda burner, as shown in Fig. 2.2. Fig. 4.2 shows the molar concentrations at the output of the steam reforming reactor for a steam-to-carbon (S/C) rate of 3.

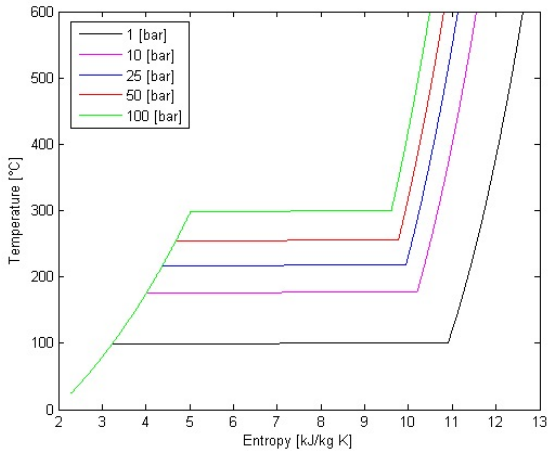


Fig. 4.1: T-s diagram for isobar vaporizations

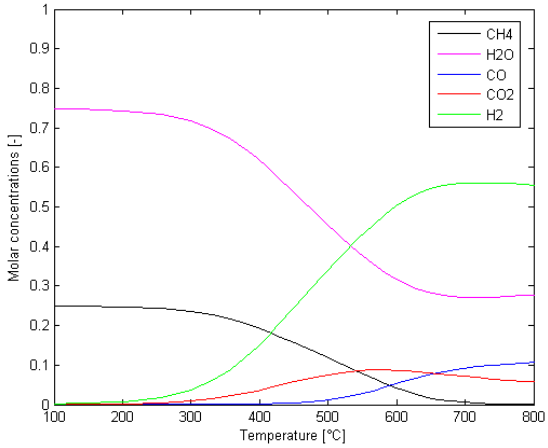


Fig. 4.2: Molar concentrations of steam reforming

After the modeling and design of FC-CHPs a few system simulations were conducted and compared to the simulation of a conventional heating installation. Table 4.1 shows the most important parameters of the FC-CHP (FC: fuel cell, PLH: additional peak load heater). Table 4.2 shows the settings for the conventional heating installation. Table 4.3 shows the prices used in the simulations to be discussed next.

The total efficiency of the fuel cell is 84%, which is quite low compared to other publications (Harrison, 2004 / Wallmark et al., 2002). Nevertheless, system simulations show the advantages of the FC-CHP compared to a conventional heating installation. This validates this technology's advantages over conventional heating installations, even for systems that are not fully developed. Fig. 4.3 shows the costs and CO_2 emissions for a complete year, split into spring, summer, fall and winter and with a differentiation between weekdays (WD) and weekends (WE), as well as for the whole year. The results show that a FC-CHP may save up to 27.5% of costs (operational costs, not taking possible higher maintenance costs into consideration) and up to 23.3% of CO_2 emissions per year, compared to a conventional heating installation.

Table 4-1: Fuel cell micro-CHP

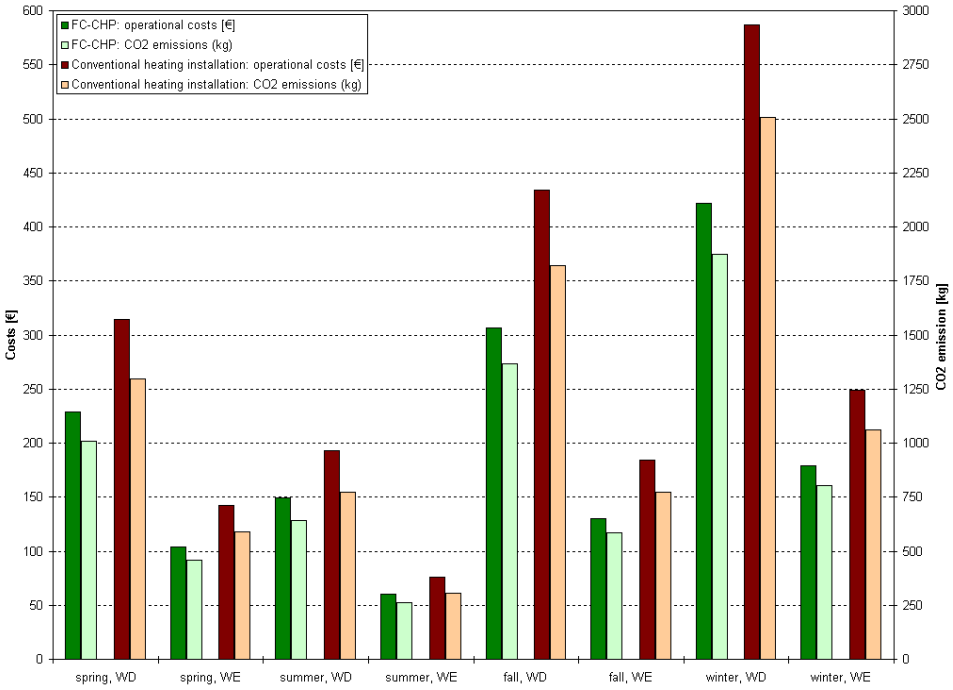
Parameter	Value
FC: min. thermal power	1.200 W
FC: max. thermal power	6.000 W
FC: thermal efficiency	60%
FC: electrical efficiency	24%
FC: minimum on-time	1800 s
FC: minimum off-time	300 s
PLH: min. thermal power	1.000 W
PLH: max. thermal power	10.000 W
PLH: thermal efficiency	85%
PLH: minimum on-time	60 s
PLH: minimum off-time	240 s
Hot Water tank: volume	750 l

Table 4-2: Conventional heating installation

Parameter	Value
Min. thermal power	4.000 W
Max. thermal power	24.000 W
Thermal efficiency	85%
Minimum on-time	60 s
Minimum off-time	240 s
Hot Water tank: volume	500 l

Table 4-3: Prices

Parameter	Value
Gas	0,05344 € / kWh
Electricity (drawn)	0,16785 € / kWh
Electricity (feed back into grid)	- 0,09 € / kWh



Entire year

FC-CHP:
- Costs: 1580.87 €
- CO_2: 7000.90 kg

Conv. heating installation:
- Costs: 2031.54 €
- CO_2: 9127.90 kg

Comments
Operational costs only (maintenance costs excluded)

Gas price for all systems without any petroleum tax reduction

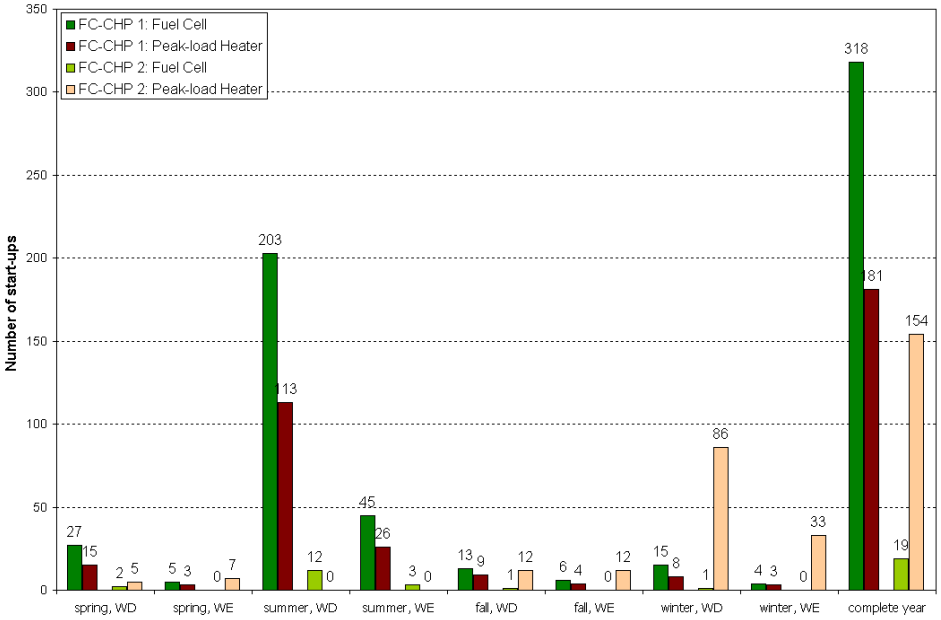
Abbreviation key
WD: weekday (Mon – Fri)
WE: weekend (Sat, Sun)

Fig. 4.3: Costs and CO_2 emissions of a FC-CHP and a conventional heating installation

As discussed above, an important issue concerns identifying areas with a high potential for optimization to guide future development. By varying parameters and re-running system simulations, we can demonstrate the influence of parameters such as efficiency, maximum power, degree of modulation (lowest possible power for a given maximum power) as well as the control strategy (also denoted by energy management).

The durability of current fuel cells is still limited and is highly affected by the number of times they are started up and shut down (start-ups and shut-downs). A great deal of research activity therefore focuses on optimizing the fuel cell life-cycle. Additionally, it is worth-while to concentrate on the energy management of FC-CHPs, since this considerably affects the number of start-ups and shut-downs, respectively.

Fig. 4.4 shows the comparison of a FC-CHP with a simple energy management (FC-CHP 1: controlled by heat demand only) and an intelligent energy management (FC-CHP 2: considering the season, outdoor temperature, current heat demand, predicted upcoming energy demand, etc.). The results show that introducing an intelligent energy management can reduce the costs and CO_2 emissions slightly (3.9% and 3.7%, respectively, per year). Simultaneously, the number of start-ups and shut-downs of the fuel cell can be reduced significantly from 318 per year down to 19 per year, which is a reduction of 94.0% and will considerably extend the life span of the fuel cell.



Entire year

FC-CHP 1:
- Costs: 1645.34 €
- CO_2: 7267.30 kg

FC-CHP 2:
- Costs: 1580.87 €
- CO_2: 7000.90 kg

Comments
Operational costs only (maintenance costs excluded)
Gas price without any petroleum tax reduction

Abbreviation key
WD: weekday (Mon – Fri)
WE: weekend (Sat, Sun)

Fig. 4.4: Number of startups of FC-CHP with simple and intelligent energy management

CONCLUSIONS

Thermodynamic and system simulations can significantly speed up the design, evaluation, analysis and optimization of micro-CHPs. Simulation is thus an important tool for engineering and development and can contribute to the improvement of micro-CHPs.

In this paper we have presented the simulation tools being developed and have discussed the results obtained from investigating fuel cell micro-CHPs. The results not only confirm the advantages of this technology over conventional heating installations, but also serve to identify the benefits and shortcomings of each technology. Further-more, we have shown that simulations can be used for rapid and simple analysis and optimization of micro-CHPs and guide future development.

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