DYNAMIC MODELING OF WÄRTSILÄ 5 kW SOFC SYSTEM

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ABSTRACT

The dynamic modeling of the 5 kW SOFC system with all balance of plants components, valves, measurement devices, heat recovery and control systems are presented. The modeling is based on the actual test-rig designed and constructed recently by Wärtsilä Corporation. The main purpose of such dynamic modeling is to collect basic understanding of system behavior during different operating phases such as load changes, shut-down, start-up, air-fuel ratio, etc. Such information is essential before designing a complete system which is going to operate stand-alone. The results from dynamic modeling help to prevent some unforeseen characteristic that may harm the system. During the transient behavior of the SOFC system, one is also interested in controlling the system by some key parameters such as stack temperature, pre-reformer operational temperature and burner temperature. The study describes basic design criteria and properties of the test system. Characteristics of major subsystems such as fuel and air supply, steam supply, exhaust heat recovery, back-up power, power electronics and control system are also explained.

INTRODUCTION

In August 2002, Wärtsilä Corporation and Haldor Topsoe A/S entered into a cooperation agreement to start a joint development program in planar SOFC technology. This program aims to bring highly efficient, clean and cost-competitive fuel cell products to the market in the power range above 200 kW. The products will be designed for both stationary power generation and marine applications. Within the program, a conceptual study of a 250 kW planar SOFC system for CHP applications was presented in 2003 (1) along with strategies to counteract stack ageing (2). The present study investigates a dynamic calculation model of the 5 kW system constructed by Wärtsilä based on the principles presented in the conceptual study.

The test system was started with one 1.2 kW stack on September 16, 2004. The first continuous test-run had duration of 1080 hours. Generated power was supplied to the Finnish national grid. System was shut-down in order to change and test new balance of plant components. Four new 1.2 kW stacks are planned to be installed in February 2005 bringing the peak electrical power up to 5 kW. Meanwhile, testing will continue with one 1.2 kW stack. The 5 kW stack will be installed after preparing this manuscript.

Practical applications for fuel cell systems are obviously the best way of testing the viability of a particular system. Nevertheless, for advancing the knowledge on these systems, computational models can be very helpful. For understanding the system level
interactions and their implications on system performance and in model-aided controller design, system level dynamic models of fuel cell power plants built from physics based component models are extremely useful. Additionally, system level dynamic models also help in evaluating alternative system architectures in an integrated design and control concept.

SOFC POWER PLANT SYSTEM

The SOFC system under consideration is based on the Wärtsilä test system built during 2004. The plant is a natural gas fuelled power system including all the balance of plant (BoP) components, fuel processing units, measurement devices, control facilities (valves, Programmable Logic Controller (PLC)) and grid connection devices (DC/DC converter, DC/AC invertors, etc.). The BoP components in the system consist of a fuel pre-heater, desulphurization reactor, pre-reformer, anode pre-heater, SOFC stack, catalytic burner, air pump, cathode pre-heater, two heat recovery heat exchangers, steam generator and a super heater. The sulphur components are removed in a desulphurization reactor from in the pressurized natural gas and which is then reformed in a pre-reformer before entering the stack. The reformer is a fixed bed reactor where all higher hydrocarbons are converted with steam into methane, hydrogen and carbon oxides. The steam required in the steam-reformer is supplied from an external steam generator. The SOFC system with all its BoP components is presented in Figure 1.

In addition to the stack, BoP components and water management described above, purge gas for start-up, power conversion, measurement devices and control systems are also included in the modeling as has been provided in the test system. These systems are not shown in Figure 1.

Figure 1. Basic flow sheet of the SOFC system without control system and grid load.

Cathode air is supplied by a blower and preheated in a heat exchanger before entering the stack. The cathode off-gas after preheating the air is used as oxidant in the catalytic burner. A preliminary dynamic calculations of the system showed that the air after recuperator (E3) may not be enough to burn all the fuel in the catalytic burner under some circumstances, therefore an additional line is included into the system which ensure the air supply into the burner, see the dashed line.

In addition to the stack, BoP components and water management described above, purge gas for start-up, power conversion, measurement devices and control systems are also included in the modeling as has been provided in the test system. These systems are not shown in Figure 1.
THE APROS PROGRAM

APROS simulation software developed by VTT provides tools, solution algorithms and model libraries for full-scale modelling and simulation of dynamic flow processes, such as different combustion power plants. Besides the process, automation and electrical systems can also be modelled. The model libraries have been comprehensively validated against real physical process experiments. The model libraries of APROS cover a comprehensive set of process plant components, such as pipes, valves, pumps, heat exchangers, reactors, and tanks. The thermal hydraulic solution in the program is based on mass, momentum and energy balance in one-dimensional as shown below

\[
\frac{\partial \rho}{\partial \tau} + \frac{\partial \rho V}{\partial z} = 0 \tag{1}
\]

\[
\frac{\partial \rho V}{\partial \tau} + \frac{\partial \rho V^2}{\partial z} + \frac{\partial \rho}{\partial z} = S \tag{2}
\]

\[
\frac{\partial \rho H}{\partial \tau} + \frac{\partial \rho VH}{\partial z} = S \tag{3}
\]

where \( A, \rho, V, H, \tau, z, S \) are area, density, velocity, enthalpy, time-scale, direction and source term respectively. The numerical solution is based on a general finite-volume technique with staggered grid arrangement. The SIMPLE scheme algorithm is employed to handle the pressure-velocity coupling. The governing equations are discretized and then the non-linear terms are linearized as is usually done in CFD (Computational Fluid Dynamics) but in one-dimensional theory. Fluid properties such as conductivity and volumetric heat capacity are provided as a function of temperature. For two phase flows, APROS can also be used with a 6-equations two-fluid model or a 5-equations drift-flux model (phase velocities). Boiling, condensation and critical wall heat flux based on several different correlations are other useful features in this simulation program.

SOFC MODELING

A simplified SOFC cell model has been developed from the works of (3-4) which is a zero-dimensional steady state model based on an adiabatic energy balance. The model is validated against one-dimensional numerical model and available experimental data. In the model different ways to regulate the air-rate and fuel-rate is used to achieve a specific power output, as described below:

1) Fuel and air are provided to the cell at a constant rate and then the fuel utilization and the cell temperature which vary depending on the load (or current) can be calculated.

2) Fuel and air flows are manipulated to maintain a constant fuel-utilization for a prescribed average cell temperature.

3) Fuel and air rate flows are varied to maintain a constant cell voltage at a prescribed average cell temperature.

The first method which is a feed-backward method is simpler than the two other methods which can be called as feed-forward method. However, thermal cycling of the cell would
lead in situations with load increase and then there would be risk for carbon formation due to cooler temperature of the cells.

The Area Specific Resistance (ASR) is extracted from the known characteristic curves available in the literature. Minimum values of the ASR are described by a polynomial function of temperature. However, two different exponential forms with functions of temperature are also available.

Four stacks with 75 cells in each of them are provided in the present study which is based on the actual SOFC plant. The total electrical output of the four stacks results in 5 kW.

**FUEL PROCESSING**

Fuel processing for the SOFC plant consists of both hydro-desulphurization and a fuel pre-reformer. Natural gas is filtered and fed into the fuel processing system using a standard mass flow controller. Both the fuel cell and the pre-reforming catalyst are very sensitive to sulphur and therefore any sulphur compounds have to be removed to a very low levels in the desulphurization reactor before entering the pre-reformer and the stack. This reactor has minimal effect on key operating conditions such as temperature and pressure because it is primarily used to remove trace amounts (parts per million, ppm) of sulphur compounds and therefore. The desulphurization process occurs in a fixed bed reactor operating at about 300°C. This reactor consists of two separate heating zones which are also considered in the present modeling. Since the chemical reactions taking place within desulphurization reactor neither generate heat nor consumes heat, same temperature is maintained in both zones. The heat losses are neglected in this reactor as well as all the other components.

As the fuel needs to be preheated to more than 600°C, any hydrocarbons in the natural gas at this temperature level will tend to form olefins, which are very strong carbon precursors, and have to be removed before entering the stack. This can be accomplished by steam reforming of hydrocarbons at lower temperature (around 500°C) in a simple adiabatic reactor, pre-reformer. The pre-reformer utilizes the heat content of the feed steam to drive the steam-reforming reaction by the use of a highly active nickel catalyst which can promote the steam-reforming reactions at low temperatures. The pre-reforming reactions result in an equilibrium gas mixture containing hydrogen, carbon monoxide, carbon dioxide, methane and steam as per the reactions of the model given below:

\[
\begin{align*}
\text{CH}_4 + \text{H}_2\text{O} &\leftrightarrow 3\text{H}_2 + \text{CO} \\
\text{CH}_4 + 2\text{H}_2\text{O} &\leftrightarrow 4\text{H}_2 + \text{CO}_2 \\
\text{CO} + \text{H}_2\text{O} &\leftrightarrow \text{H}_2 + \text{CO}_2
\end{align*}
\]

The performance of the pre-reformer is directly reflected by the temperature rise/drop across the reactor depending on the type of feed. For the fuel processor model the following assumptions have been made:

- Axial plug-flow, pseudo-homogenous reactor for the reforming gases.
- Concentration and temperature gradients in radial direction are neglected (i.e. 1-dimensional model).
• Heavier hydrocarbons are gradually hydro-cracked to methane.

The reaction rates, partial pressures of the gas components and other necessary data are taken from the literature; see (5-7). Pre-reformer has inlet and outlet heating zones as well as three adiabatically controlled zones around the catalyst bed, which are also considered in the calculation model. These elements compensate the heat losses form the reactor. In the real test there exist some heat losses from this reactor while such heat losses are neglected in the calculation.

**BALANCE OF PLANT**

All the balance of plants equipments, such fuel processing (desulphurization reactor, the pre-reforming and the steam generation), heat exchangers, air compressor, valves (shut-off valves, control valves, etc), measurement equipments, control devices (electronic, control valves and PLC), grid connection (converter, load, etc.) are included in the model, all based on the actual data of the balance of plant components. All the components are connected to each other by pipes with actual sizes and length.

**Steam Supply**

Since anode recycling system has not yet been implemented, water is used to provide a constant steam flow for the reformer. The water is filtered, de-ionized and pressurized before supplying it into a steam generator operating at a pressure of 2.5 bar(g). The generated steam is superheated up to 500°C by an electrical heater before entering into the steam reformer. A pressure difference measurement over a measuring flange is used to determine the rate of steam flow. The flow is adjusted by a pneumatic control valve in a way that steam to carbon ratio is maintained at around 1.5 (H₂O/total C) in order to avoid carbon formation in the reformer.

There have been some difficulties in obtaining a stable steam flow in modeling which is similar to the actual system. A preliminary calculation by APROS showed that the flange diameter was too low compared to the steam rate.

**Heat Exchangers**

Five plate heat exchangers are used in the modeling based actual system, which are recuperator (air pre-heater), anode pre-heater, fuel pre-heater and two heat recovery heat exchangers. In the modeling all the data from the actual heat exchangers have been included, such as plate length, mean height between the plates, number of plates, efficiency, pressure drop, etc.

The remaining exhaust heat is recovered by water cooled plate heat exchangers located at both fuel- and air-side exhaust lines. Cooling water temperature measurements and flow rates are used to determine the amount of waste heat recovered. However, in the calculation model air-cooled heat exchangers to cool down the excess exhaust heat instead of water-cooled heat exchangers. The reason for such change was that controlling the air stream showed to be much easier than controlling the water flow. The rate of the coolant flow in the heat recovery heat exchangers are controlled in way that the off-gases temperature leaving these heat exchangers is kept at 90°C. Since at both actual test and the calculation the exhaust off-gasses are cooled to the same temperature level then it does not matter whether water or air is used to cool these exhaust off-gasses.
**Air Supply**

In the model a side channel blower have been included for the system air supply. Air flow rate on the cathode side of the system is measured using a thermal mass flow meter. Automation system controls the rotational speed of the blower with a PID controller and a set point.

**Catalytic Burner**

In the system a catalytic after-burner is use for combusting the anode off-gases leaving the fuel cells. Using a catalytic burner ensures extremely low emissions with varying fuel compositions. Burner flue-gas temperature is maintained around 700 °C. In the calculation model the temperature after the burner is measured and then the air flow rate into the burner is controlled by a control valve and respective PID controllers.

**AUTOMATION AND CONTROL SYSTEM**

The calculation model has been automated with many different PLC devices similar to what has been used in the actual test system. Automation and control system includes various voltage, temperature and pressure measurements, as well as flow measurements and control of fuel, air, steam and purge gas. Fuel and air flows can be controlled according to process temperatures and stack voltages which vary according to electrical loading. The calculation model has been equipped with a significant number of shut-off valves and by-pass pipelines according to the actual test. In the modeling it has been adapted to describe these valves as similar to the actual test system as possible. Such valves in the calculation model are also used to isolate subsections of the system providing the possibility to operate different sections separately. This has been a highly beneficial feature to compare the calculation model with the actual test for different subsections. Concentration of combustible gases is monitored at many different points in order follow the chemical reactions taking place in different parts.

In addition to these system controls, a back-up control system for emergency shut-down situations is also provided. Back-up control will ensure safe shut-down of the system under any circumstances. In addition, similar to what has been used in the actual test a hardwired emergency shutdown sequence of the whole system is included in the calculation model in case of failures which damage the system or cause danger to surroundings.

**POWER ELECTRONICS**

In the test system, the voltage generated by stacks is transformed up to a range of 595 - 650 V using DC/DC converters. This high voltage DC current is then transformed into a three phase 400 V current by a line inverter. After the inverter, voltage is connected to a standard 50 Hz grid through an LC filter and an isolating AC/AC transformer. The line inverter detects frequency and amplitude of the grid voltage using a special algorithms and the inverter synchronizes the output voltage to the detected grid voltage.

Since in the calculation model we do not have access into the actual grid connection, these steps are simplified into a grid connection with 5 kW constant loading. The load is defined with both active and reactive parts (about 53 degree) according to usual electrical
equipments. The line inverter protection hardware and software are thus neglected in the calculation model. The DC/DC converters and DC/AC inverters are defined with several features such as grid frequency, efficiency, nominal power, nominal voltage, maximum power, maximum ampere, ratio of DC to AC voltage, gain of AC controller, etc.

RESULTS

At the time this paper was being prepared, there were no results from the 5 kW test system (the system was running with 1.2 kW stack). In order to show how the model self-adjusts during some parameter changes the following results are shown. The initial temperature values of the system are shown in Fig. 1 which corresponds to the stable, long running time. All the set points are taken from the heat balance calculation of the system from other programs. It should be noted that the APROS program is suitable for an existing system to be analyzed and it is not suitable for designing a heat balance scheme to be developed. Therefore, the heat balance scheme was developed by other program and the flow arrangements such as fuel and air flow are taken from the calculated heat balance scheme. However, if the real system does not work as supposed (and expected) as from the beginning, due to several operating facts, then the set-points might not be good choices for the system. It is thus highly desirable to develop a system that self controls and adjusts itself based on the operating system. This can be achieved by intelligent control system (ICS). Such investigations are also a main objective of such dynamic study. In it, heat losses from the system are neglected and the attention is paid on the system behavior instead.

![Figure 2. Initial values.](image)

The predicted fuel utilization and el-efficiency at the initial stage (through the given set-points) are shown in Fig. 3. The fuel utilization is predicted to be about 0.6 which is much lower than the expected. This issue together with the flow set-points causes the el-efficiency to be almost zero which can be seen in Fig. 3 also. Since the fuel utilization is less than expected, the air flow supplied to the system is expected to be larger than...
needed in relation to the fuel supplied. The initial value for the air supply was 110.8 kg/h. Therefore, the air supply is reduced gradually to reach a value that is suitable for the fuel supplied without changing any other value or damage to the other components. A dynamic self-control system must respond to this value change until it reaches a stable operation.

Figure 3. Initial values for utilization factor and el-efficiency (%).

In Fig. 4 the air supply is reduced to 70 kg/h (from the initial value of 110.9) and the control systems successfully adjust the system to this new value after about 1500 seconds. The cathode inlet temperature oscillates around the 670°C which is the required temperature value for both cathode and anode sides. Due to less air flow, the electric power required from the element is much lower than the initial stage and the cathode temperature oscillates around 670°C until the control components adjust the system to this new value. The inlet anode temperature does not change very much since the fuel supply remains the same as in the initial value, which is also shown in Fig. 4. Because the air supply is a cooling source for the stack then the stack temperature must increase when the air supply is decreased. This is also shown in Fig. 4. The stack temperature is increased from about 740 to about 760. This new stack temperature is still under the design limit.

Figure 4. The self-adjusted values for anode, cathode and SOFC temperature after 1500 seconds.
Consequently, the electrical efficiency is increased because the heating demand from the electrical element is reduced which can clearly be seen in Fig. 5. The el-efficiency is increased from 0.05% to about 25% which is a notable change. In addition, it should be mentioned that if the fuel utilization increases to higher values then the el-efficiency will also increase to more than 40%. The fuel utilization depends strongly on the stack and its environment (including the flow distribution) and does not change significantly if the air flow is changed, which is also shown in Fig. 5.

Figure 5. The self-adjusted values for the utilization factor and el-efficiency after 1500 seconds.

It might be interesting to see how the system behaves during the first seconds when the air supply is reduced. These can be seen in Figs 6 and 7.

The stack temperature is increased to about 780°C after one second and then decreased to around 760°C and remains almost constant. This mostly due to the fact that the electrical element which was adjusted for a higher air-rate cannot suddenly respond to a reduced air-rate and the air temperature at the cathode side increases suddenly to about 690°C and in turn increases the stack temperature. However, the provided control devices with their measurement tools begin to react very fast and control the system soon after the new value for the air flow supplement. The fuel utilization decreases somewhat while the electrical efficiency increases suddenly to oscillate around 20% after only 2 second until it reaches to a stable value when the system stabilizes, see Fig. 7.
Figure 6. The self-adjusted values for anode, cathode and SOFC temperature during the first 10 seconds.

Figure 7. The self-adjusted values for the utilization factor and el-efficiency during the first 10 seconds.
CONCLUSIONS

The dynamic modeling of the Wärtsilä SOFC is presented with all equipments, such as the stack, heat exchangers, burner, pre-reformer, desulphurization reactor, considerable amount of measurement devices, many different control valves, shut-off valves, grid connection units, etc is presented. The calculation modeling is adapted to be as similar as the actual test system designed recently by Wärtsilä Corporation. While the pressure drops, pipe sizes and other features are considered to be as similar as the actual system, the heat losses are neglected in the present study, in contrast to the test system.

It has been found that beside automation and choice of proper BoP components, it is very important to design a system which is fully self-controlled in terms of air and fuel flow-rates. The system characteristics such as electrical efficiency depend strongly on a proper self-controlled system. In the soon future it would be possible to compare the dynamic model with the actual test system when the 5 kW stack is installed (1.2 kW at the time when the present study was prepared). The dynamic model can be used to study several different flow configurations and system improvement.

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