2008-01-01

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FUEL CELLS 2008
Science & Technology

Introduction

Conventional power generation plants are based on the steam turbine (Rankine) or gas turbine (Brayton) cycle, thus the thermal efficiency of these plants is restricted by the Carnot principle [1]. Advanced gas turbine combined cycle plants can achieve up to a maximum thermal efficiency of 60%. By contrast, predicted results for integrated solid oxide fuel cell (SOFC) and gas turbine systems have shown thermal efficiencies of 70% or higher [2].

SOFCs are considered one of the most promising energy conversion devices, since they can achieve very high electrical efficiencies, with low emissions and good reliability [3]. In the context of climate change, increasing energy conversion efficiency, and energy security SOFCs are likely to play an important role in the production of electricity.

The tubular SOFC configuration, developed by Siemens Power Generation, Inc (SPGI) formerly Siemens-Westinghouse, is considered to be the most advanced and is approaching commercialisation.

In industry there is a need for SOFC models that are easily calibrated to match the continuous and rapid technological advances in the field. Also the models should have short computational times. The objective of this work was to develop a model of a SOFC stack flexible enough for use in industry, that could accurately predict SOFC performance under various operating conditions and using a range of fuels.

Aspen plus, a process simulator that is widely used in industry, was used to model the SPGI tubular SOFC stack. The model, which is based on Gibbs free energy minimisation, performs heat and mass balances and considers the ohmic, activation and concentration losses for the calculation of the SOFC operating voltage.

Data available in the literature on the SPGI 100 kW AC tubular SOFC stack, polarisation curve, stack exhaust composition and temperature etc., will be used to validate the model. In a future study this SOFC stack model will be integrated with a biomass gasifier model and balance of plant models all developed in aspen plus.

Methodology

SOFC stack description

The 100 kW SOFC stack was the first field unit to utilise the seal-less cathode supported cell (22 mm diameter, 150 cm active length, 834 m^2 active area) and in stack reformers [4]. A simplified schematic of the stack is shown in Fig. 1. It employs 1152 cells in 48 bundles of 24 cells each [5].
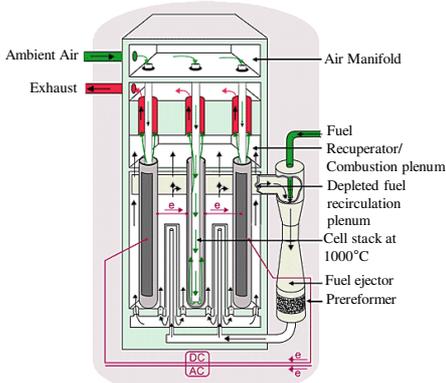

Fig. 1 Simplified schematic of a SPGI SOFC stack [6]

The cell geometry used is as follows: cell length 150 cm, outer diameter 22 mm, anode thickness 0.1 mm, cathode thickness 2.2 mm, electrolyte thickness 0.04 mm, interconnection thickness 0.085 mm, and interconnection width 9 mm [7 , 8].
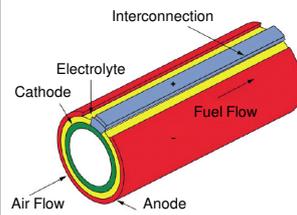

Fig. 2 depicts a schematic of a single tubular cell. The closed end of the tube is not shown, this can be seen in Fig. 1.

Fig. 2 Schematic of a single cell tube [5]

Process simulation software

Aspen plus was chosen to model the system. It is a steady state chemical process simulator, which uses unit operation blocks, models of process operations. The user places these blocks on a flowsheet, specifying material and energy streams. An extensive built in physical properties database is used for the simulation calculations. The program uses a sequential modular approach.

There is no built in model that can represent a SOFC. A common approach is to develop a complete SOFC stack model in a programming language (Fortran etc.), and link it to aspen plus as a subroutine [9]. The subroutine must incorporate complex phenomena such as chemical/electrochemical reactions, and heat and mass transfer, making them difficult and time consuming to develop and use. This type of model would not achieve the objectives of this research. An alternative method proposed by Zhang et al. [9], using existing aspen plus unit operation blocks with minimum requirements for linking of a subroutine, was used.

Modelling

Fig. 3 depicts the aspen plus flowsheet of the SOFC. Each component or section is clearly defined and may be compared with the real system shown in Fig. 1.

The inlet fuel pressure is set by a design specification using an assumed fresh fuel/fuel cell pressure ratio. The inlet pressure must be sufficient to drive the anode recycle process.

The preformer is assumed adiabatic. 'Cooler1' decreases the temperature of the preformer outlet gas simulating the edothermicity of the steam reforming reactions. A design specification varies this temperature until the heat stream 'Q2' equals zero, i.e. adiabatic.

It was assumed that at the anode the carbon monoxide (CO) shifted to hydrogen (H_2) and the methane (CH_4) was reformed to H_2, so that only H_2 reacted electrochemically [10].

Oxygen (O_2) is separated from air in the cathode and is fed to the anode, simulating the O_2 ion crossing the electrolyte to the anode side.

The amount of depleted fuel recirculated is set using an assumed steam to carbon ratio.

Complete combustion of the remaining fuel occurs in the combustion plenum.

Equations reported by Song et al. [11] were used to calculate ohmic loss, taking into account realistic electron/ion paths, please refer to Fig. 4. The resistivity of each SOFC component (anode, cathode, electrolyte and interconnection) was determined as a function of operating temperature [12]. Achenbach's [13] semi-empirical correlations were used for determining the activation loss. Both ordinary and knudsen diffusion were considered for the calculation of effective diffusion coefficients and the equations derived by Chan et al. [1] were implemented for the calculation of the concentration loss.
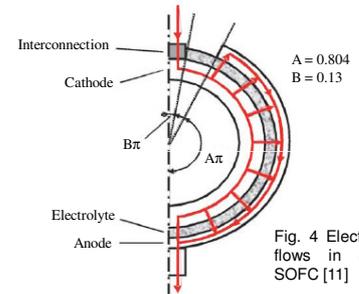

Fig. 4 Electronic/ionic flows in a tubular SOFC [11]

Fig. 5 depicts the polarisation curve of the SPGI tubular SOFC. Similar curves are reported in other sources [10, 14]. This curve and other data, such as stack exhaust gas composition and temperature will be used to validate the model.
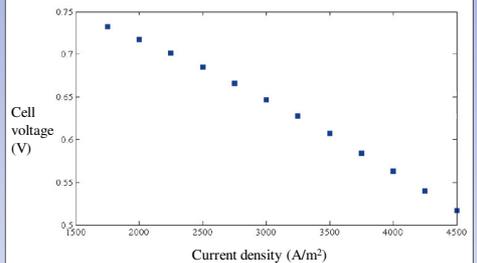

Fig. 5 SPGI tubular SOFC polarisation curve [15]

Conclusions

A computer simulation model of the Siemens Power Generation, Inc solid oxide fuel cell stack, utilising their air electrode supported tubular design, was developed using aspen plus.

The model outputs expected results with regard to stream composition compared to SPGI data, the most notable being the anode outlet stream and the stack exhaust. The calculated preformer outlet temperature and stack exhaust temperature from the model are in good agreement with SPGI data.

Due to problems with the voltage model calculations the model is not yet fully validated. Once these problems are overcome, detailed sensitivity analyses will be done.

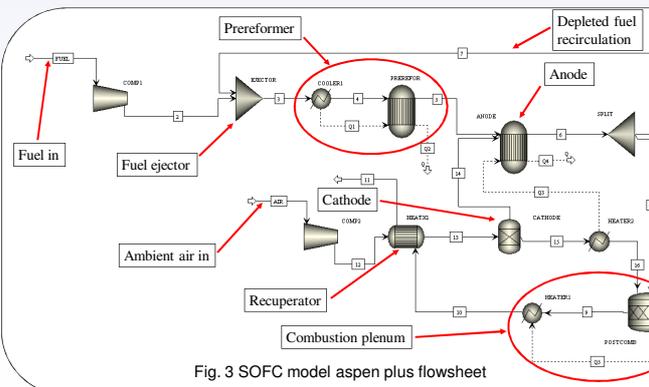In a future study this SOFC stack model will be integrated with a biomass gasifier model.

Fig. 3 SOFC model aspen plus flowsheet

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