Investigation of Processes in the "Reformer-Fuel Cell" System by the Mathematical Modeling Method

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Introduction

In the context of increasing demand for renewable energy sources, fuel cells represent a highly efficient, clean, and sustainable energy conversion source. Fuel cells can be divided into six different categories depending on the types of electrolyte and fuel used. Among them, solid oxide fuel cells (SOFCs) attract significant attention due to their high efficiency, cost-effectiveness, and ability to use various types of fuel, in addition to hydrogen, such as hydrocarbons, coal gas, alcohols, ammonia, etc. Despite achieving comparable current densities with hydrogen, some degradation issues caused by these types of fuels affect the long-term stable operation of SOFCs.

Mathematical model of SOFC

In the Ansys Workbench software, a grid with tetrahedral cells totaling 55 million was created. The quality of the grid was 0,979. The computational grid was built using mathematical equations for the conservation of mass and charge, substance transport, heat exchange, ionic and electronic charge balance. Then the computational grid was processed in "ANSYS-Mesh". It should be noted that the model is planar with 30 channels. By trial and error, it was found that orthogonal quality of about 0,95 was sufficient for accurate calculations in the "ANSYS-Fluent" module.

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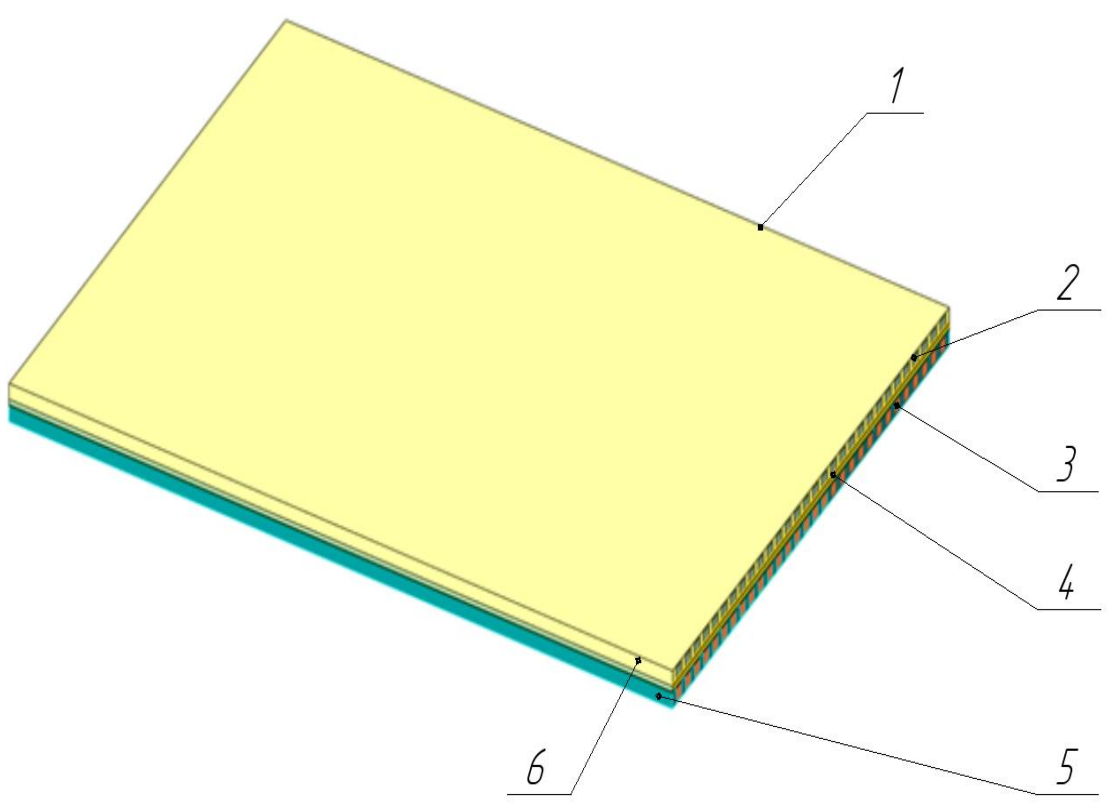

Figure 1. 3-d model of a 30-channel planar SOFC. 1 - Interconnection; 2 - anode channels; 3 - cathode channels; 4 - electrolyte; 5 - cathode; 6 - anode

Mathematical model of steam reforming system

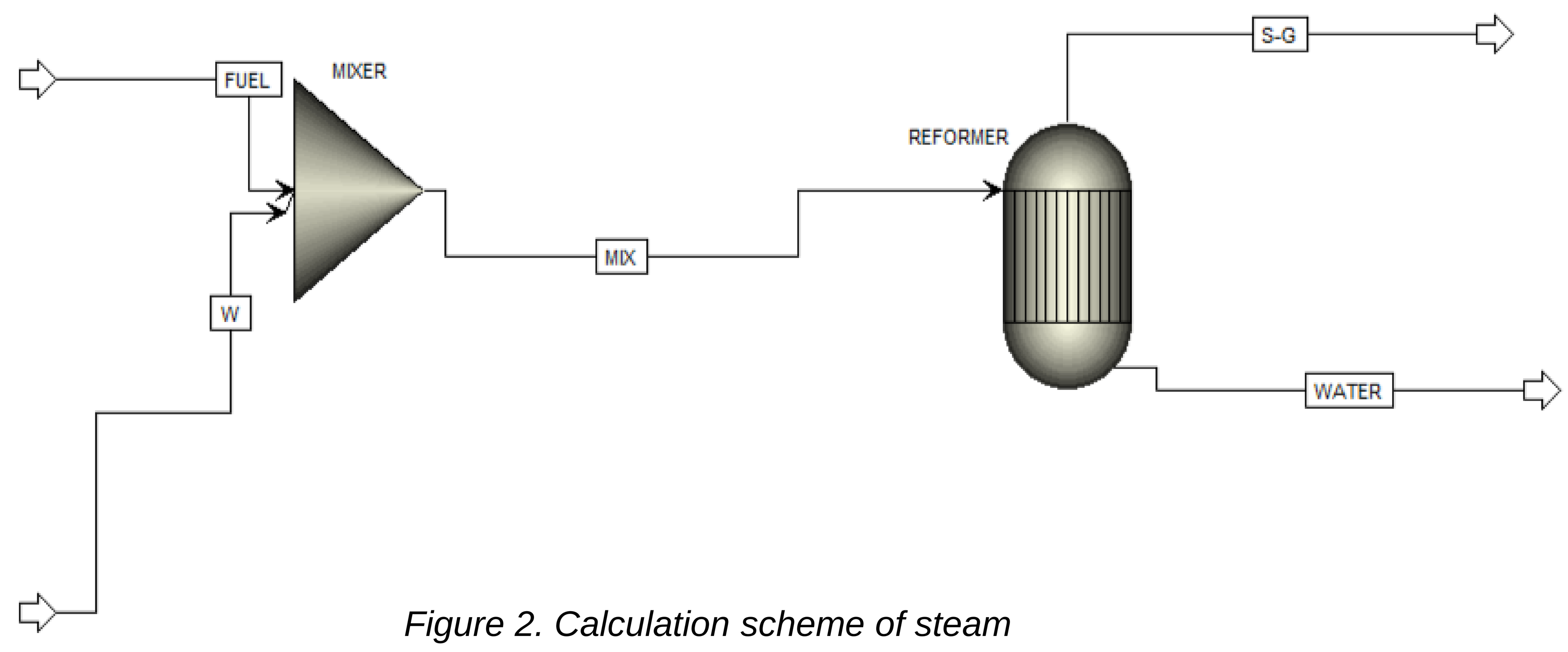

Figure 2. Calculation scheme of steam reforming system in "ASPEN PLUS" program

In the first stage, the formation of the calculation scheme was carried out which includes the following streams: the stream of the original fuel (fuel gas), the stream of water vapor (w), the mixture stream (mix), the streams of the liquid (water) and gaseous phase of synthesis gas (g-s). A mixing block and a chemical reaction reactor block were also used.

Results (I)

Element	Research fuel mass fraction, %
O_2	0,588
N_2	4,101
H_2	3,868
CH_4	21,3
C_2H_6	19,063
C_2H_4	3,217
C_3H_8	23,37
C_3H_6	3,599
C_4H_{10}	17,33
C_5H_{12}	3,538
Sum of C_6	0,92
Sum of C_7	0,22
CO_2	0,745
H_2S	0,3991

Table 1: Initial fuel composition

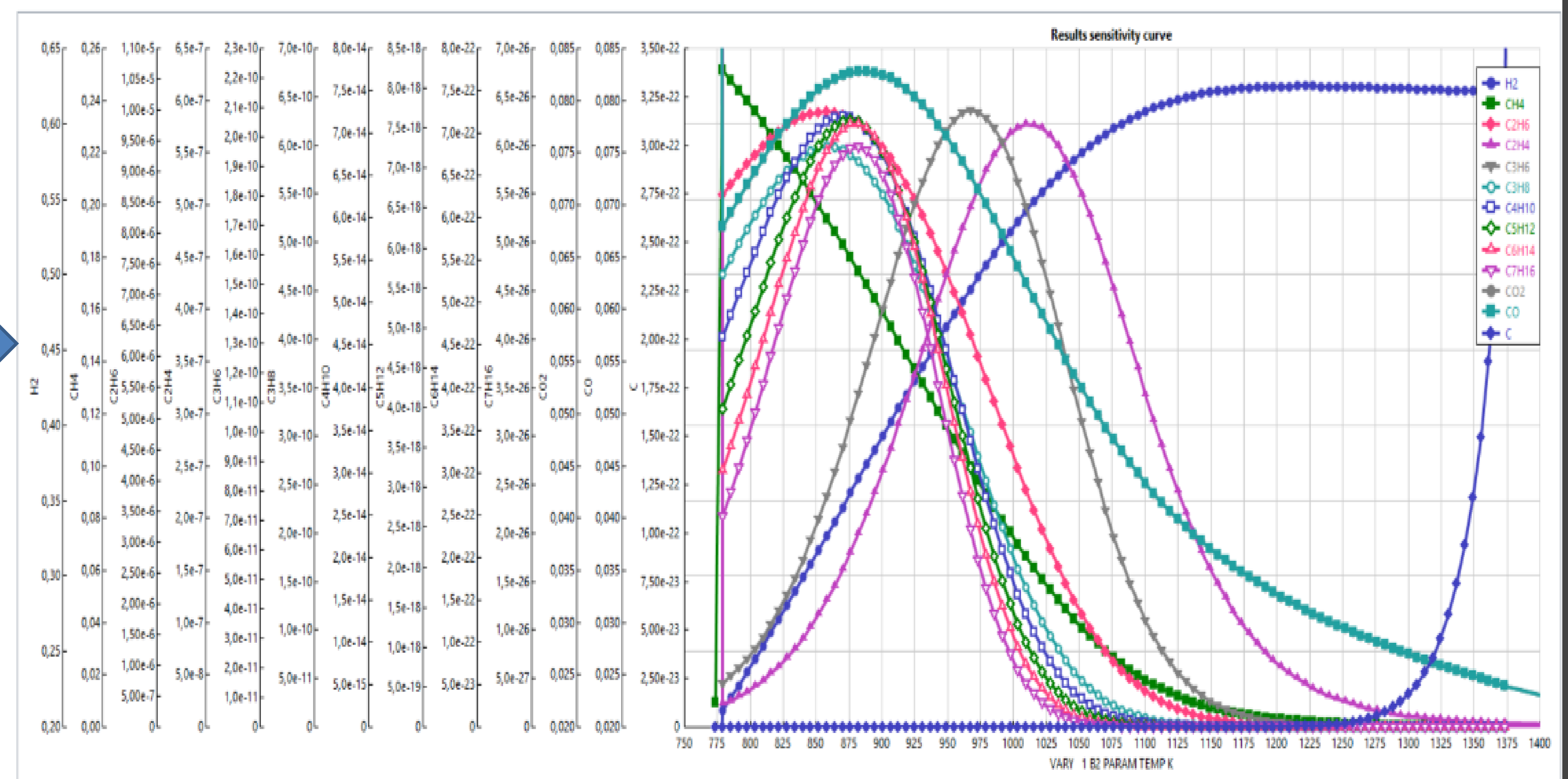

Figure 3. Result of calculation in the "ASPEN PLUS" program

Results (II)

$$\eta_e = \left(0.0000539 * \sum_{i=1}^{i} {Q_{li}}^{s-g} \times \mathrm{x}_i + 0.0000539(T_i - 20) \times \sum_{i=1}^{i} c_i^{s-g} \times \mathrm{x}_i\right) /$$
$$(0{,}0000154 * \textstyle\sum_{i=1}^{i} {Q_{li}}^{t-g} \times \mathrm{x}_i + 0.0000385 \times H_{H2O} + 0{,}0000154(400-20) \times \sum_{i=1}^{i} c_i^{s-t} \times \mathrm{x}_i + Q)$$

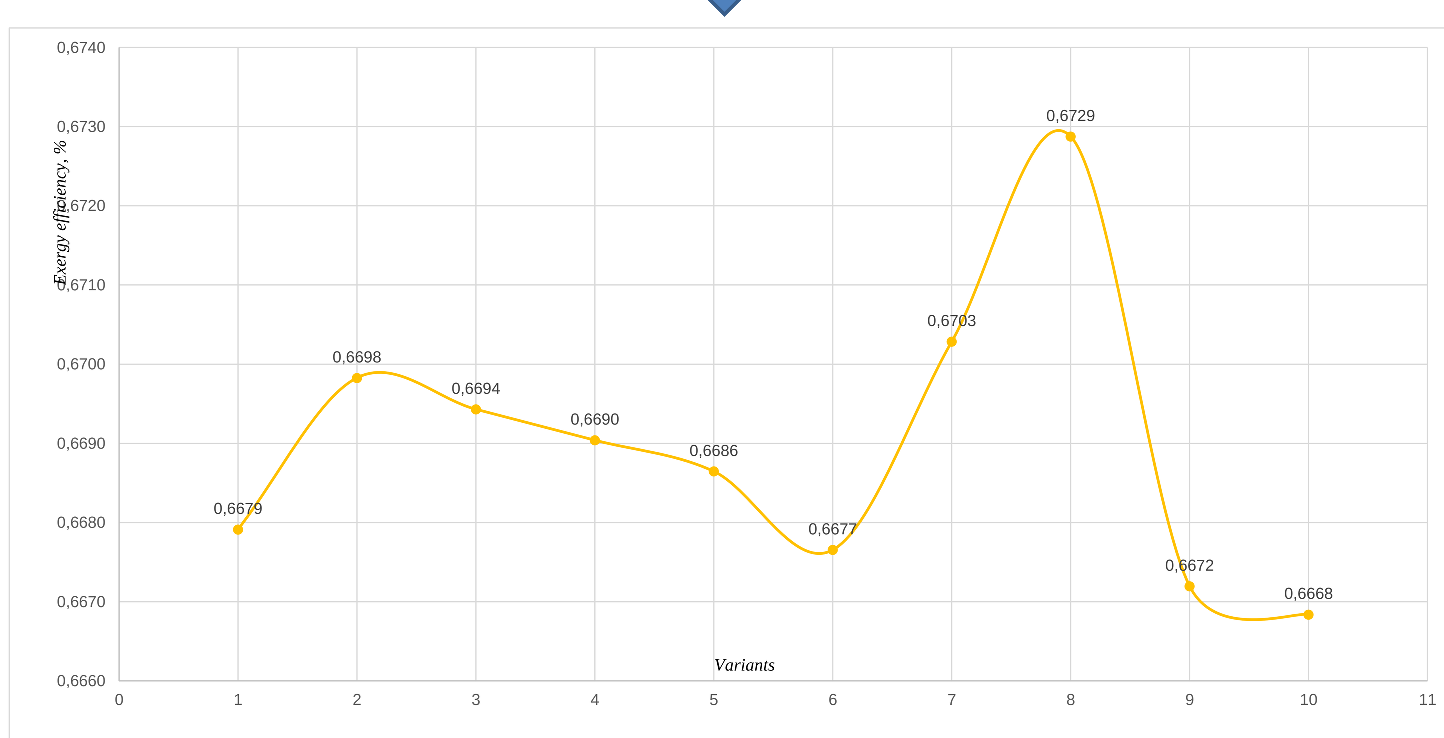

Figure 4. Exergy efficiency dependence to reformer based on composition of synthesis gas.