Modelling, optimisation and analysis of tubular high temperature solid oxide steam electrolysis cell.

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Thermomechanical and fluid dynamics analysis and design of high-temperature steam electrolysis cell based on solid oxide dense electrolyte

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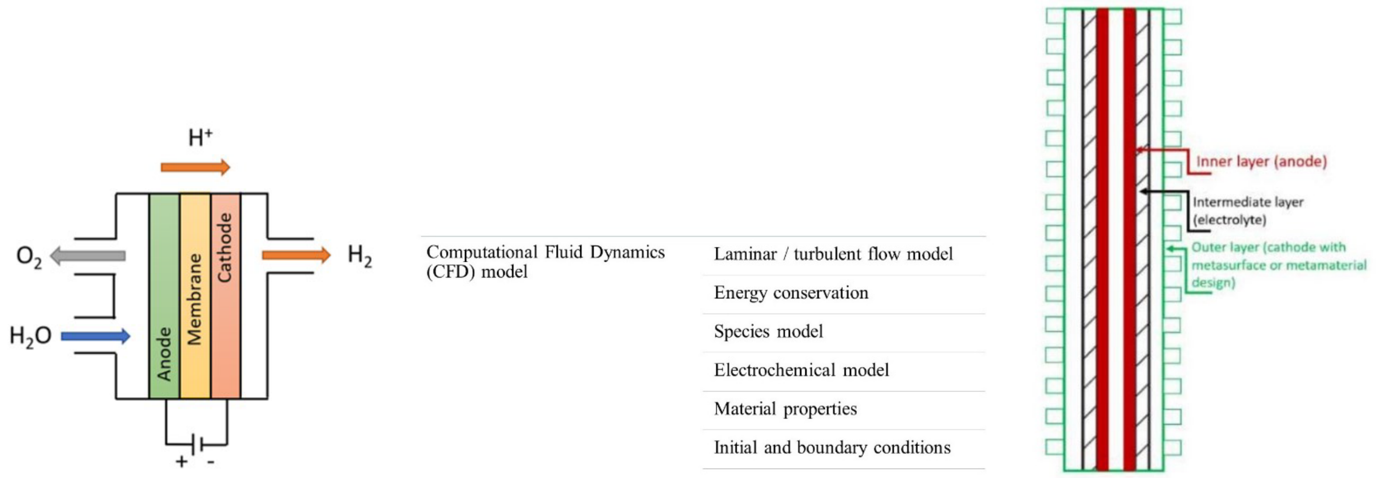
High-temperature solid oxide steam electrolysis (HT SOSE) technology stands out for its efficiency, due to the transformation of the heat energy and electricity into hydrogen, instead of a pure electricity basis [1, 2]. The use of solid materials only for all functional layers, involved in the electrochemistry, also leads to the lower cell volume and lower production and operation costs. The electrolysis process based on the solid electrolyte involves the formation of oxygen ions out of the high-temperature steam and passage of these anions through the dense membrane, as in Fig. 1(a). At the same time, hydrogen cations are consolidated at the cathode, so they do not cross the electrolyte layer, and the reduction reaction here leads to the formation of hydrogen molecules which then exit the gas channel with the remainder of the steam flow. Inert gases, such as argon, are often used as additional fluid carrier materials for either gas channel [3].



(a) (b) (c)

Fig. 1. Design of solid oxide electrolysis cell: (a) schematic cell where three chemical reactions occur during the high-temperature solid oxide steam electrolysis process; (b) sub-models of the CFD methodology for SOSE simulations; (c) main functional layers of the solid oxide electrolysis cell with a metamaterial layer.

Consideration of the complex high-temperature electrolysis process in modelling is closely linked to the level of detail, necessary for specific design tasks, and the scale of representing the process. Computational Fluid Dynamics (CFD) method employs a number of sub-models to simulate the SOSE process and other types of electrolysis cells, where each sub-model represents a part of the essential physics, as in Fig. 1(b). In the present research, CFD simulations and mechanical FEA, implemented in the commercial software, are used in order to design a SOSE cell of a tubular layout, with a metal support and implementation of a metamaterial layer, as schematically illustrated in Fig. 1(c). The project involves thermomechanical and fluid dynamics simulations for a range of high-temperature conditions with the goal to optimise the geometrical configuration. Another part of the project involves the material choice and manufacturing of one of the tubular design options with the internal steam channel [4]. The project is focused on the cell efficiency enhancement, characterization of functional layers and developing the experimental and modelling basis for the future design of a small stack of HT SOSE cells.

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Introduction & Opportunity

<u>High temperature solid oxide steam electrolysis (HT SOSE)</u> is an efficient and ecologically-friendly method of hydrogen production through conversion of the water substance into hydrogen and oxygen, using the heat and electrical energy.

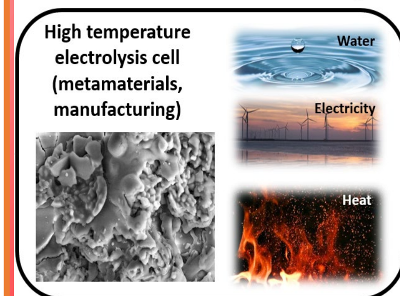
The HT SOSE is outstanding for its efficiency due to:

1) use of heat energy;
2) use of solid materials which allows reducing the cell volume;
3) reduced production and operation costs.

The SOSE technology has the most positive perspectives of integration with the existing power plants based on the nuclear or renewable energy, and also with aerospace technologies, where the excess heat and electricity is available as a byproduct.

Nuclear reactor heat & steam

Electrode & feedstocks for electrolysis

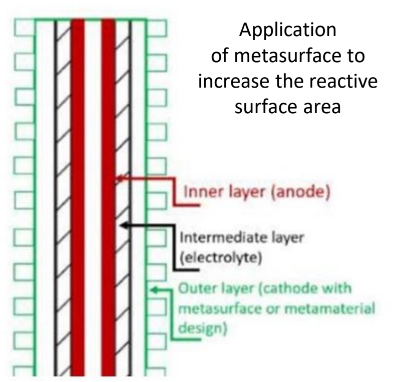


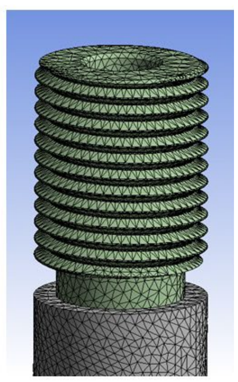
Plans, Methods & Progress

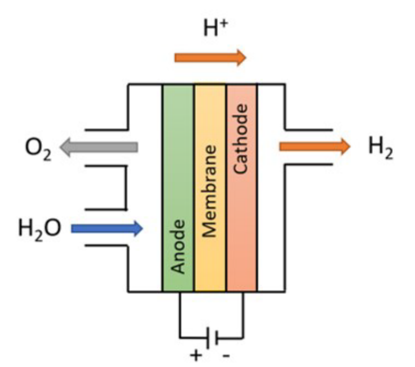
Analysis and optimisation of the tubular SOSE cell should balance the following design requirements:

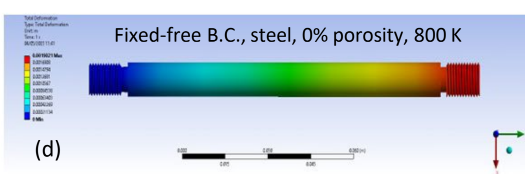
1) mechanical stability of the cell during high temperature operation;
2) electrochemical efficiency of materials, used for functional layers, where oxidation/reduction reactions take place;
3) increased surface area of the fluid – electrode interface, including the use of metamaterials;
4) efficient circulation of fluid species in gas channels;
5) convenience of manufacturing.

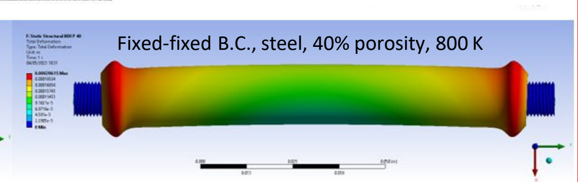
To achieve the goals, analysis of the tubular cell includes thermomechanical simulations of HT conditions and computational fluid dynamics (CFD) with the unresolved electrolyte model, species transport, laminar flow and porous materials.

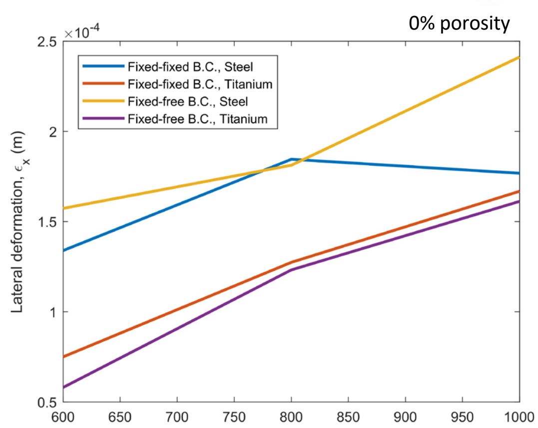


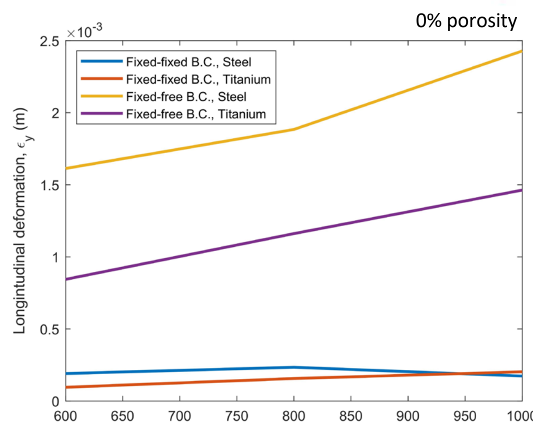


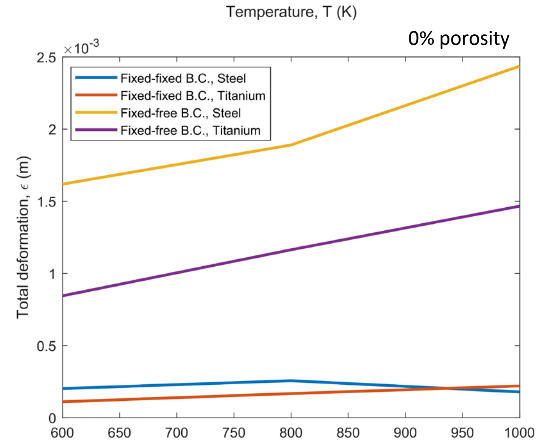


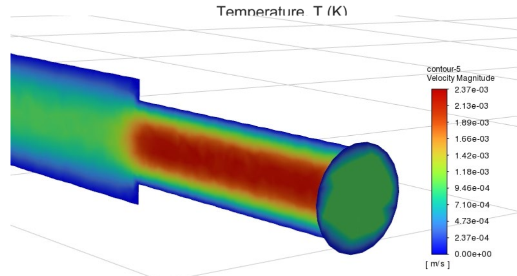


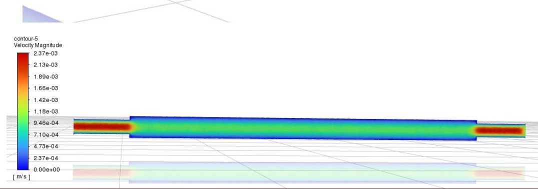












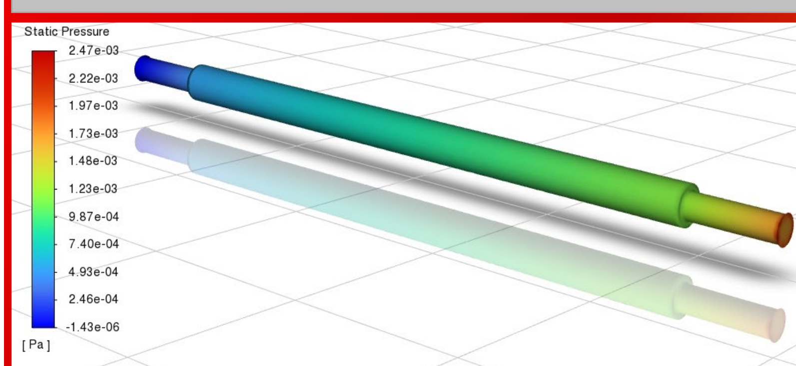
Results

Thermomechanical simulations are verified in terms of the total deformation, and considered operation conditions are:

- ✓ maximum expected 10 bars pressure;
- ✓ effect of fixed-fixed, fixed-free, fixed-elastic end conditions;
- ✓ temperatures of 600, 800, 1000 °C;
- ✓ variation of the initial substrate porosity from 20 to 40%;
- ✓ two distinct metal support materials are tested, titanium alloy and Steel 316.

CFD sub-models for the SOSE cell simulations:

- ➢ Laminar flow model, energy conservation
- ➢ Species model
- ➢ Electrochemical model
- ➢ Material models, initial and boundary conditions



Summary

Developing electrolyser cells with enhanced hydrogen production and their scalable manufacturing can play an important role in enabling not only eco-friendly development but also cost-effective, reliable, and sustainable opportunities. Thermomechanical assessments of expected deformations at high temperature bandwidth for two types of materials, used as a cell metal support were performed. Revealed changes to geometry, especially, at fixed-fixed conditions provide a basis to estimate the overall cell stability, optimise the fluid dynamics component and electrochemical performance.

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