Multi-scale Modeling of Solid Oxide Fuel Cells: from Powder to Power

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1. Solid oxide fuel cells: a multi-scale system

Solid oxide fuel cells (SOFCs) are electrochemical devices which allow a clean and efficient production of electric power at 600-1000°C. An SOFC consists of an electrolyte, which is a dense ion-conducting layer, and two porous electrodes, wherein electrochemical reactions occur (Figure 1).

SOFCs involve several chemical and physical phenomena occurring at different length-scales: the strong coupling of these processes makes SOFCs a multi-scale system.

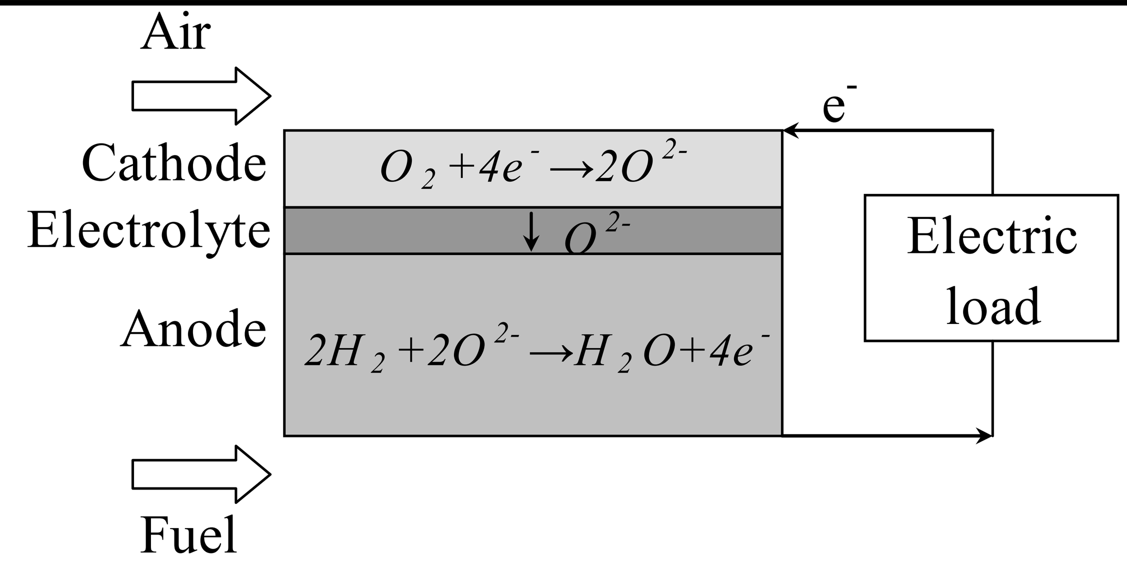

Fig. 1 - Scheme of a solid oxide fuel cell.

2. Modeling approach

We propose an integrated modeling approach, simulating both the microstructure of porous electrodes and the transport and reaction phenomena within the cell.

This approach avoids the use of any empirical, fitted or adjusted parameter: the integrated model can predict the macroscopic behavior of the cell (i.e., the power) from the knowledge of powder characteristics and operating conditions (Figure 2).

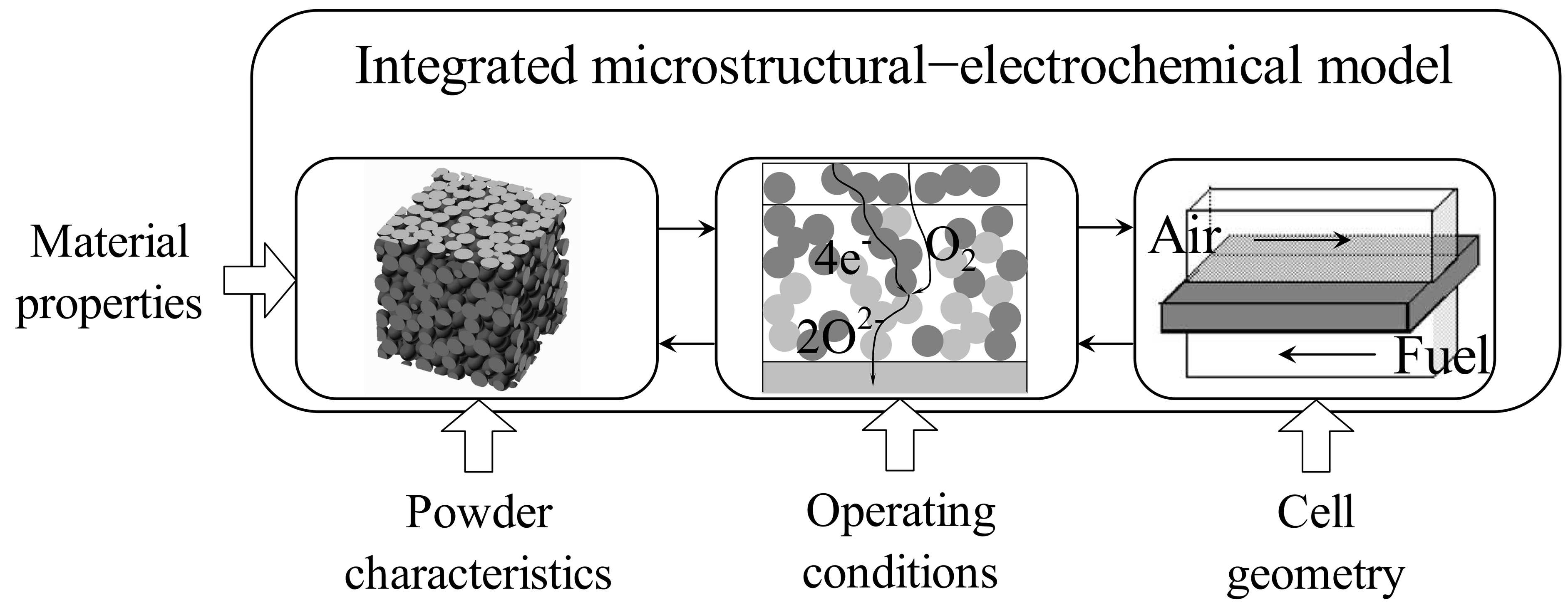

Fig. 2 - Modeling approach adopted.

3.1 Microstructural modeling

Packing algorithms are used to re-construct the microstructure of porous electrodes (Figure 3). Specific algorithms have been developed to reconstruct packings of spherical and non-spherical particles.

The effective properties are evaluated through a random-walk method and geometric analysis (Figure 4).

3.2 Electrochemical modeling

Conservation of mass and charge is applied within the cell to describe:

- electrochemical reactions,
- gas transport in the pores,
- charge transport in different phases.

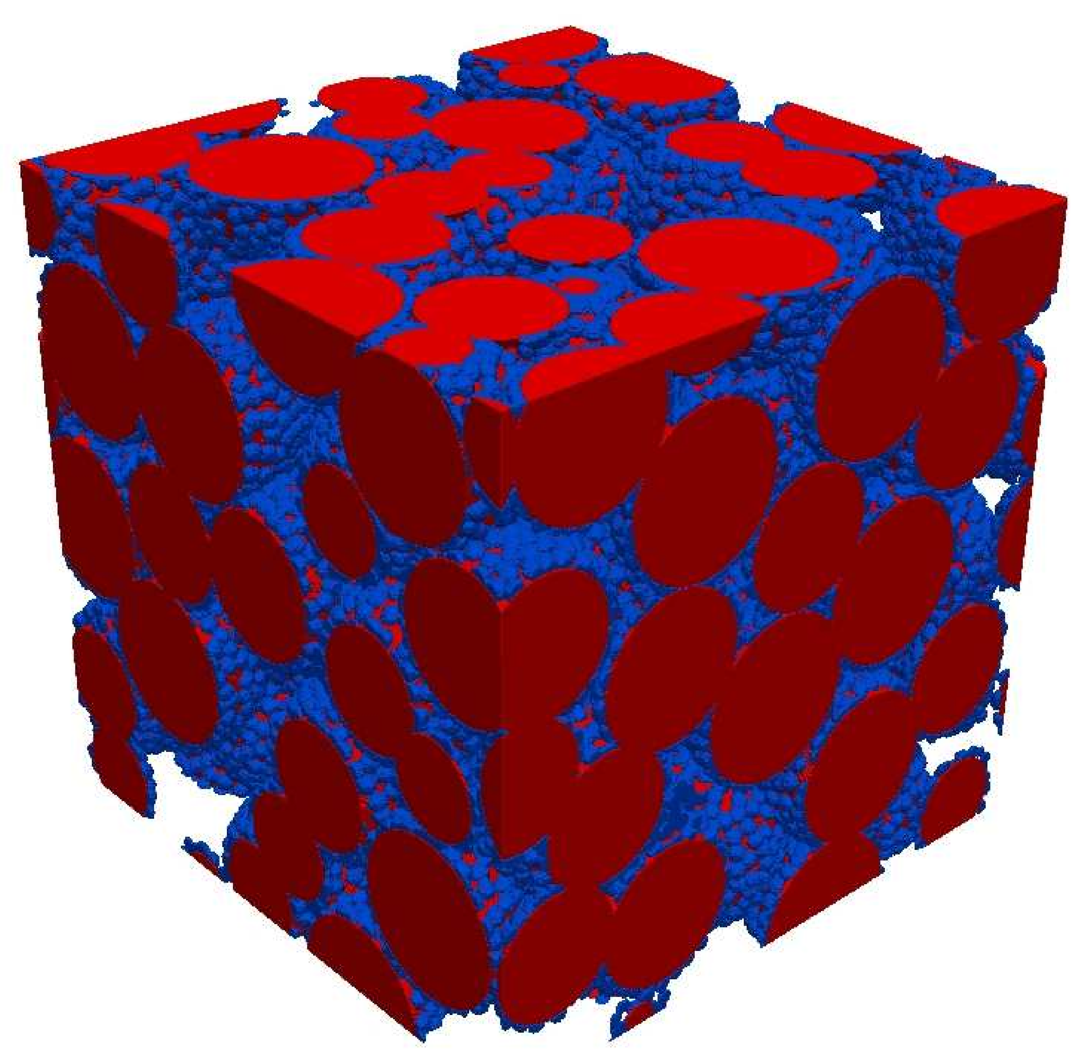

Fig. 3 - Numerical reconstruction of an infiltrated SOFC electrode.

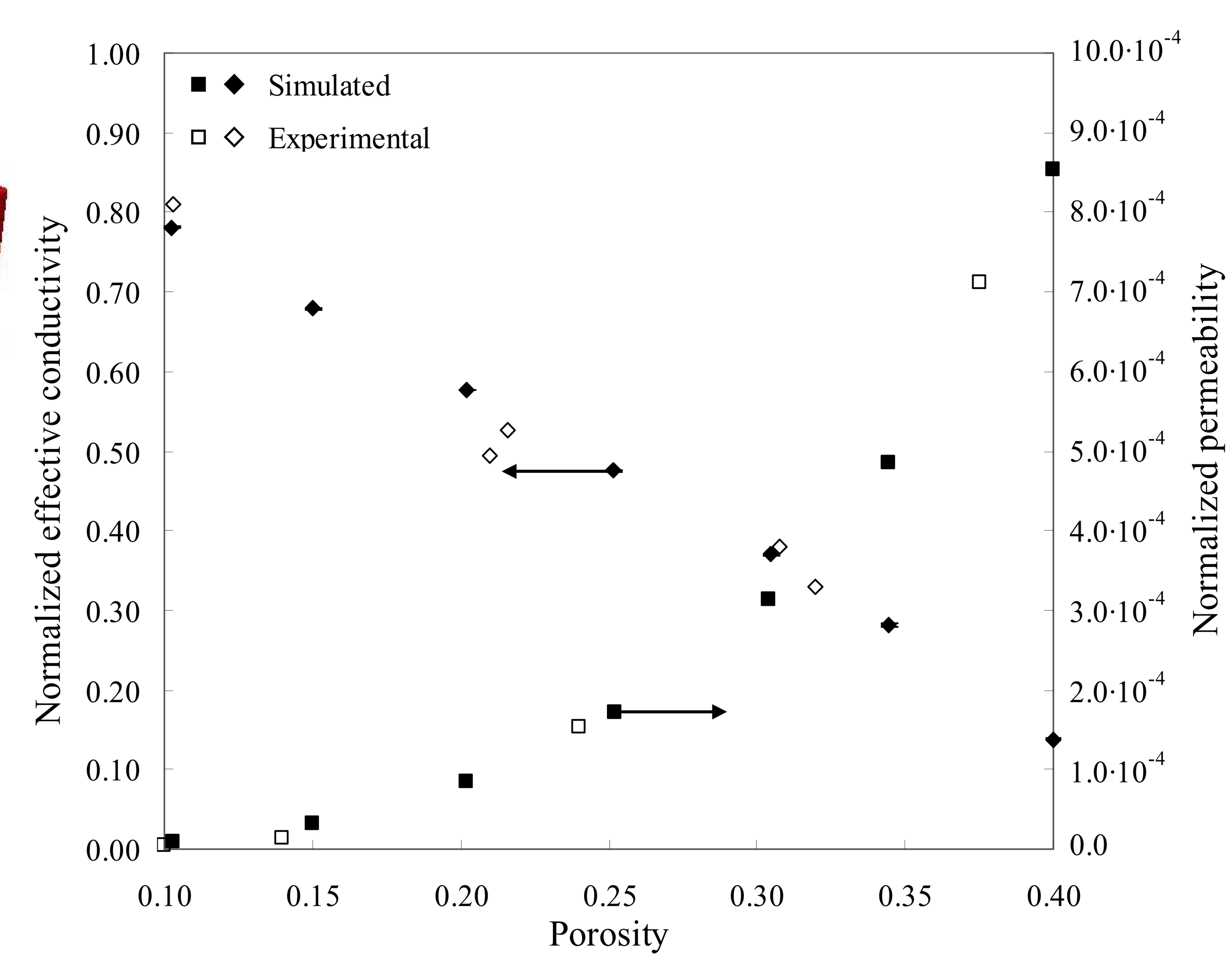

Fig. 4 - Effective properties of sintered random packings of spheres.

4. Results and applications

The integrated model is used as:

- interpretative tool of experimental data (Figure 5),
- design tool to optimize the cell performance (Figure 6).

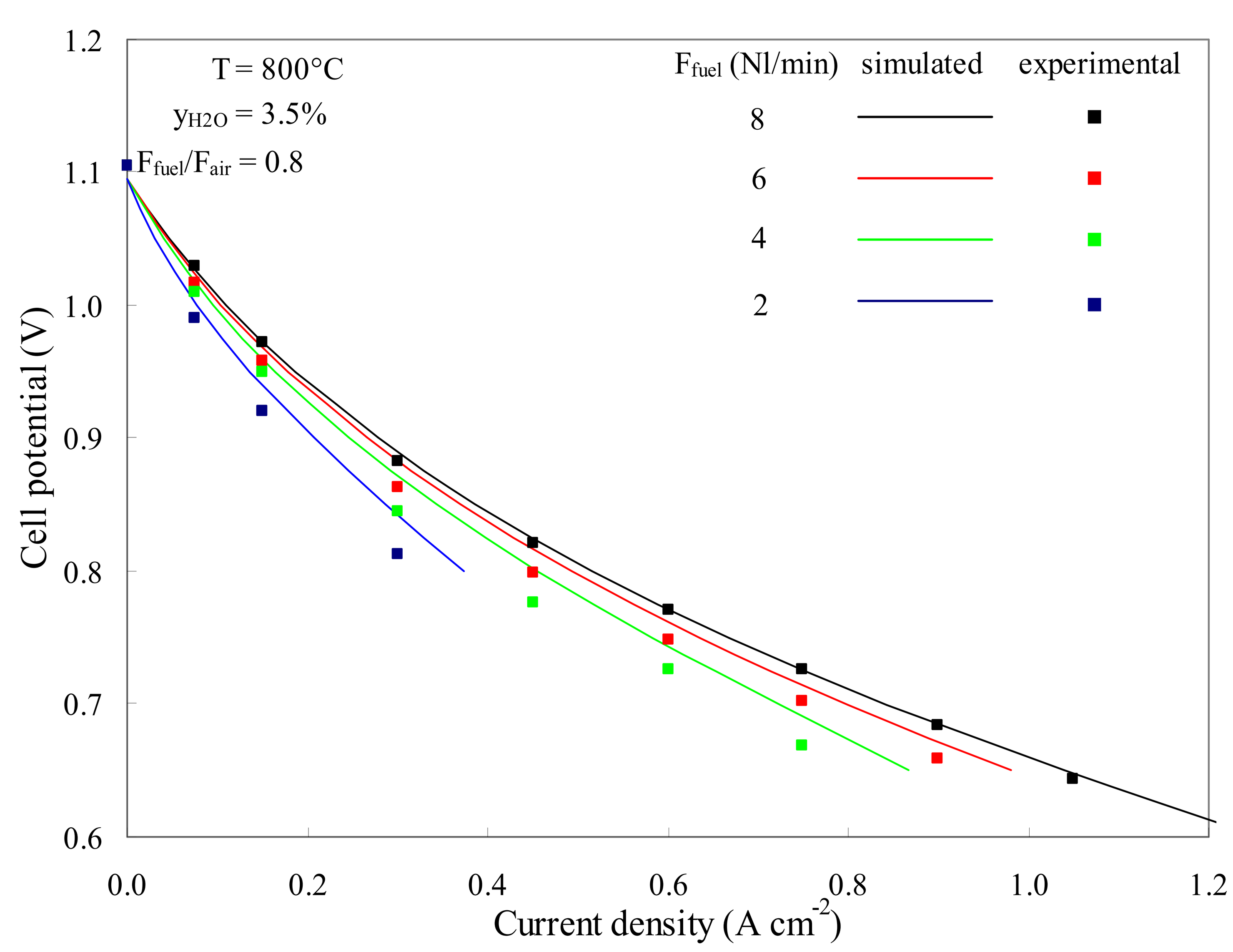

Fig. 5 - Polarization behavior of an anode-supported Jülich cell for different operating conditions.

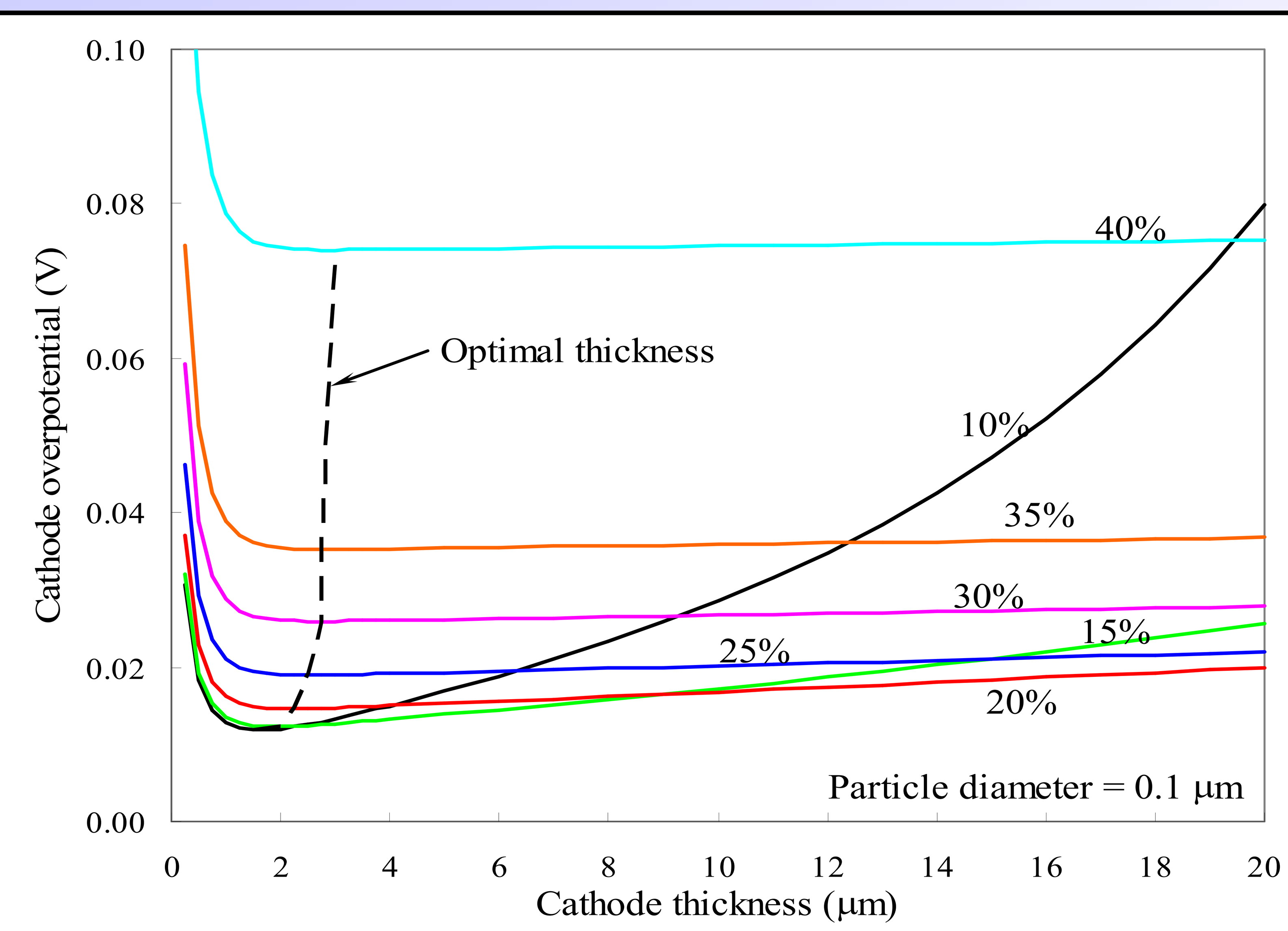

Fig. 6 - Design analysis for a composite cathode for different porosities.

References

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