

Toward predictive PEFC simulation: The importance of thermal and electrical contact resistance

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In computational models of polymer electrolyte fuel cells (PEFCs), thermal and electrical resistances between the different contacting material layers are commonly disregarded. Various experimental conductivity measurements have shown, though, that they can have a significant share in the overall through-plane resistance. Here, experimentally measured contact resistances between different MEA layers are implemented into a one-dimensional stationary two-phase PEFC model to demonstrate the importance of taking these effects into account in PEFC simulations that aim to be quantitatively predictive.

Introduction

Contact resistance (CR) is a consequence of imperfect contact between rough surfaces. Thermal and electrical contact resistance between individual layers in a membrane-electrode assembly (MEA) are known to have a large impact on cell performance and may even dominate over bulk resistance [1]. Interfacial resistance depends on the compressive load on the cell, which is applied to increase conductivity and to seal the gas flow channels. Yet, they are commonly neglected in numerical modeling of PEFCs.

Based on published experimental evidence [2–6], we argue that both thermal and electrical contact resistivities at the interfaces between catalyst layers (CLs), gas diffusion layers (GDLs) and bipolar plates (BPs) are governed by power laws with the applied clamping pressure for typical materials such as SGL and Toray carbon papers and stainless steel or graphite. These relationships are implemented into a 1D non-isothermal two-phase PEFC model to study their impact on the quantitative prediction of fuel cell performance.

Theory & experimental data

Experimental data on contact resistivity R as a function of clamping pressure P is quite plentiful in the literature for the GDL/BP interface, but varies with the materials considered. Scaling arguments for contacting fractal surfaces predict a power law $1/R \sim P^\alpha$ with exponent $\alpha \in [1/2, 1]$ depending on surface roughness and plasticity [7]. Indeed, the electrical contact resistivity between GDL and BP is well-approximated by a power law of the form [8]

$$R_c(P) = R_{c,0} \left(\frac{1 \text{ MPa}}{P} \right)^{\alpha_c} \quad (1)$$

where $R_{c,0}$ and α_c are material parameters. Also, almost all published experimental data for thermal contact at the GDL/BP interface is consistent with such a power law, as shown in Fig. 1a.

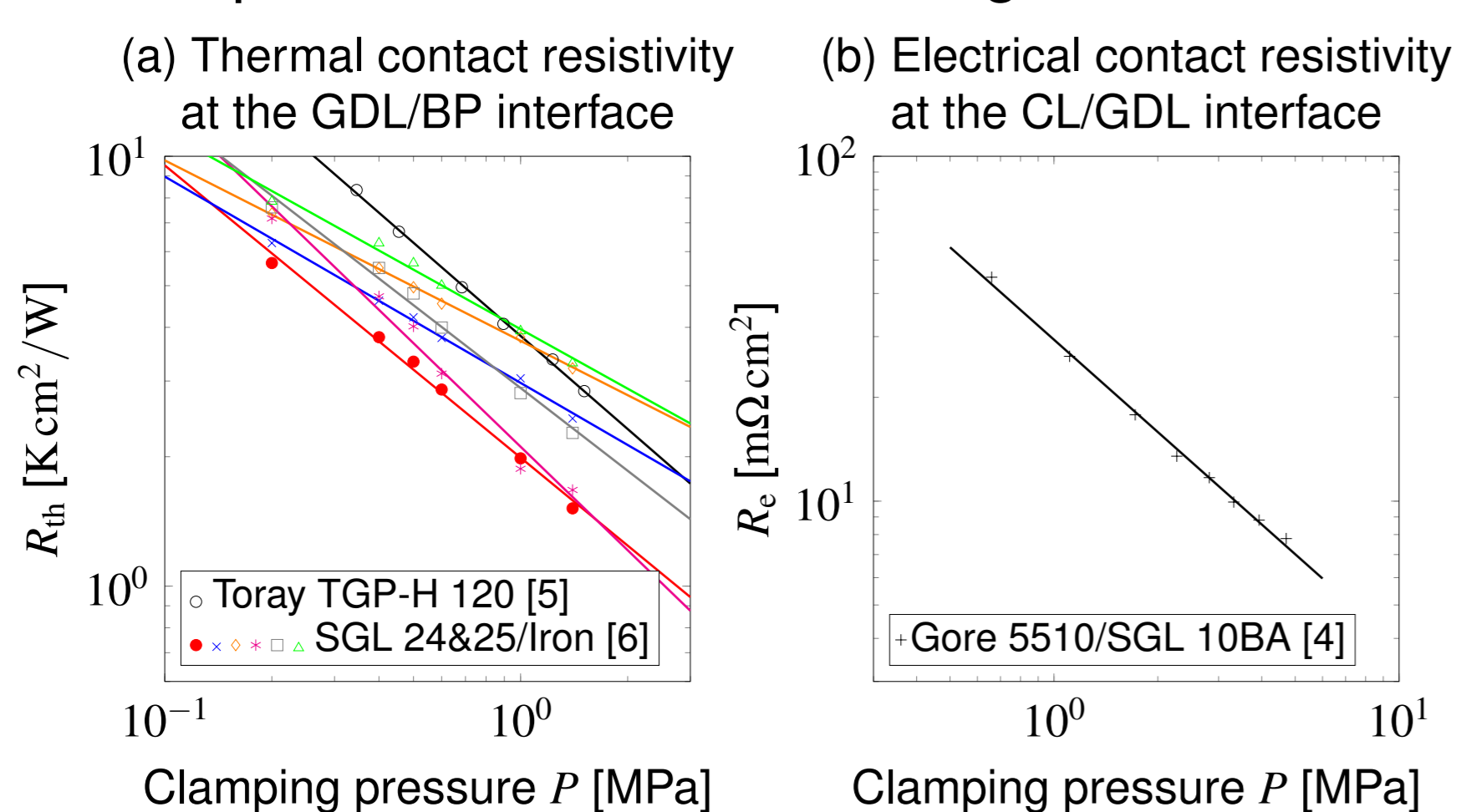


Fig. 1: Experimental data of contact resistivity as a function of applied clamping pressure. All solid lines represent individual power law fits with Eq. (1).

For other interfaces in the MEA, available experimental data is much more scarce. The electrical

contact resistivity between CL and GDL strongly depends on the presence of an MPL [4]. As shown in Fig. 1b, Eq. (1) provides a good fit to published measurements of the CL/GDL interface (without MPL). Measurements on the thermal contact between CL and GDL appear to be absent from the literature with the exception of ref. [9].

Model

We demonstrate the effect of taking thermal and electrical CR into account in modeling by implementing them into a steady-state, non-isothermal, two-phase finite element PEFC model in COMSOL Multiphysics (Fig. 2).

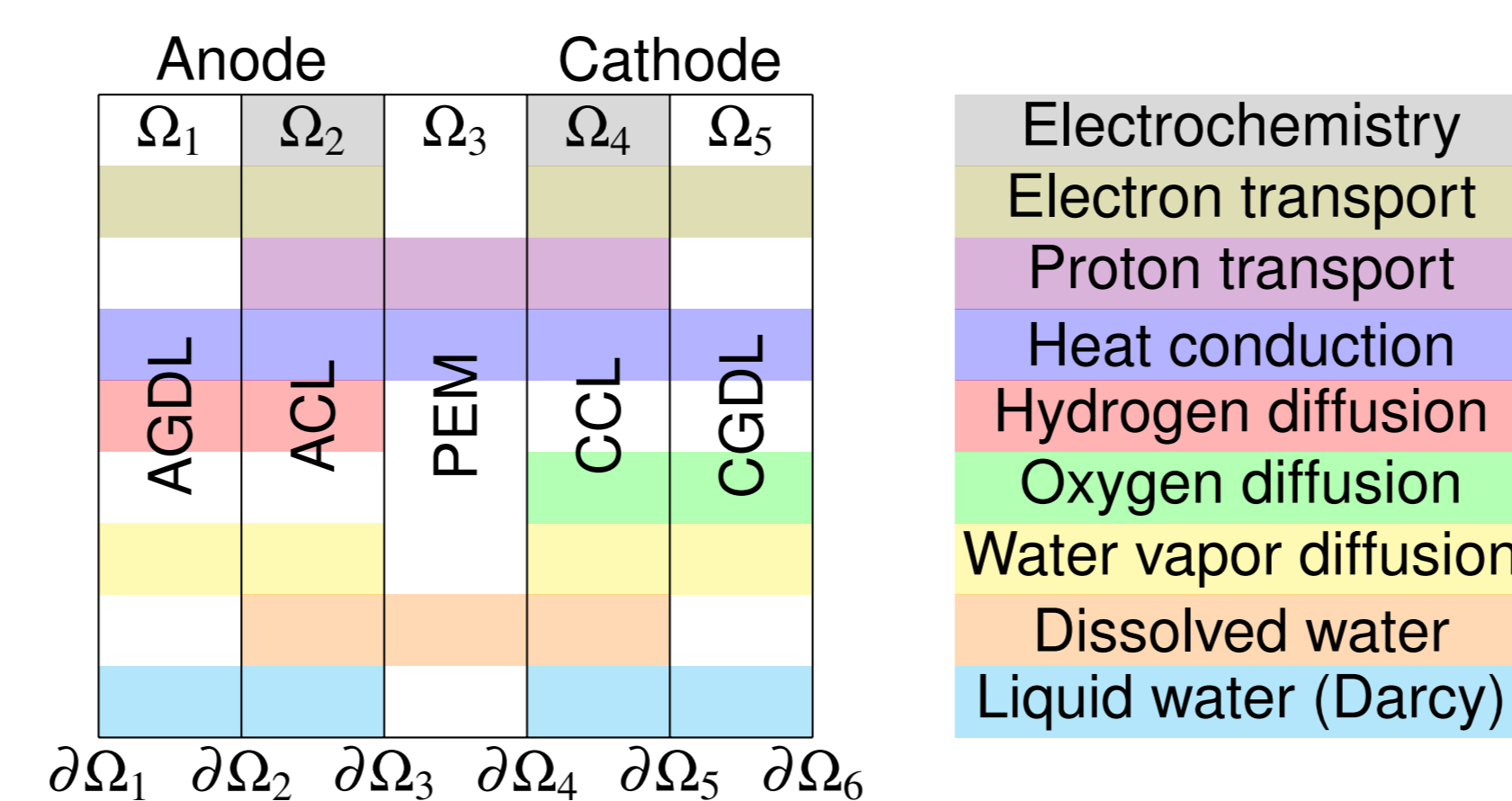


Fig. 2: Overview of the 1D PEFC model (not to scale).

Imperfect contact between any two contacting layers can be modelled by constraining the heat flux j_{th} and electron flux j_e across the interface $\partial\Omega_i$ to

$$\begin{aligned} -j_{th} \cdot \vec{n} \Big|_{\partial\Omega_i} &= \frac{T_i^+ - T_i^-}{R_{i,th}(P)} \\ -j_e \cdot \vec{n} \Big|_{\partial\Omega_i} &= \frac{\phi_i^+ - \phi_i^-}{R_{i,e}(P)} \end{aligned} \quad (2)$$

where T_i^+ and ϕ_i^+ (T_i^- and ϕ_i^-) represent the temperature and electric potential at interface i in the subdomain lying in positive (negative) direction of \vec{n} as sketched in Fig. 3. These Neumann conditions replace the continuity constraints $T_i^- = T_i^+$ and $\phi_i^- = \phi_i^+$, that are otherwise imposed.

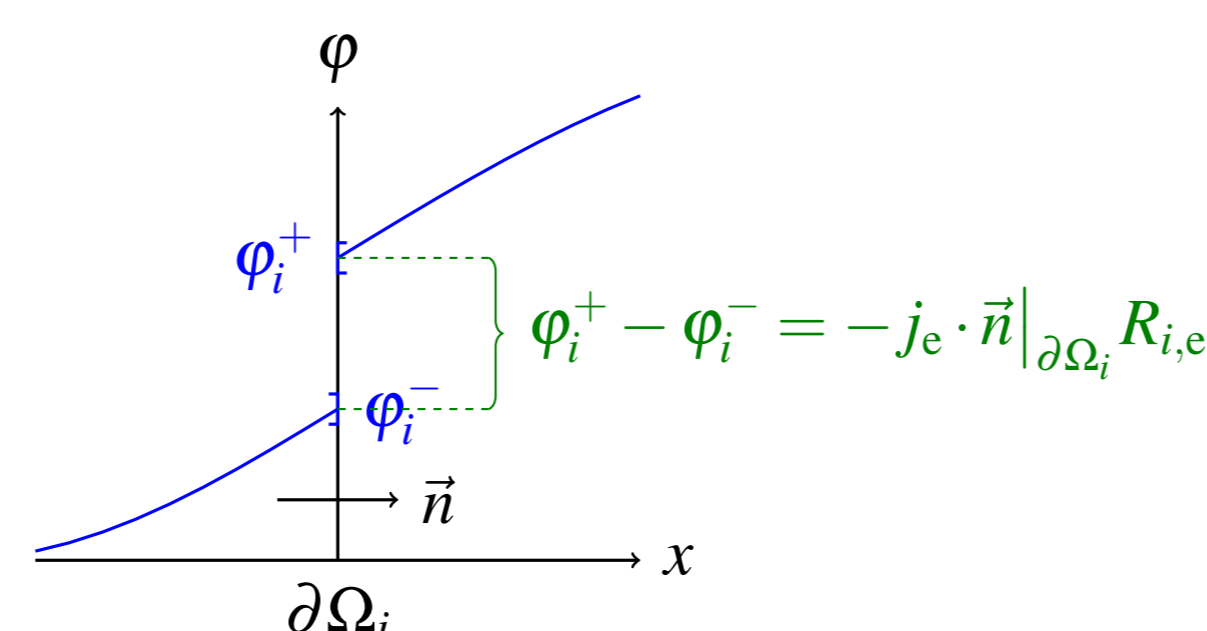


Fig. 3: Illustration of electrical contact resistance at subdomain interface $\partial\Omega_i$. x is the through-plane coordinate.

Results

A selection of simulation results with and without CR is shown in Fig. 4, obtained for the following operating conditions: Saturated hydrogen and air at 80°C and 2 bar. Thermal CR at the GDL/BP leads to a uniform increase in temperature across the cell but doesn't effect the performance notably.

On the contrary, electrical CR at the CL/GDL interface alters the electric current and thus the electrochemical reaction enough to lower the cell performance significantly.

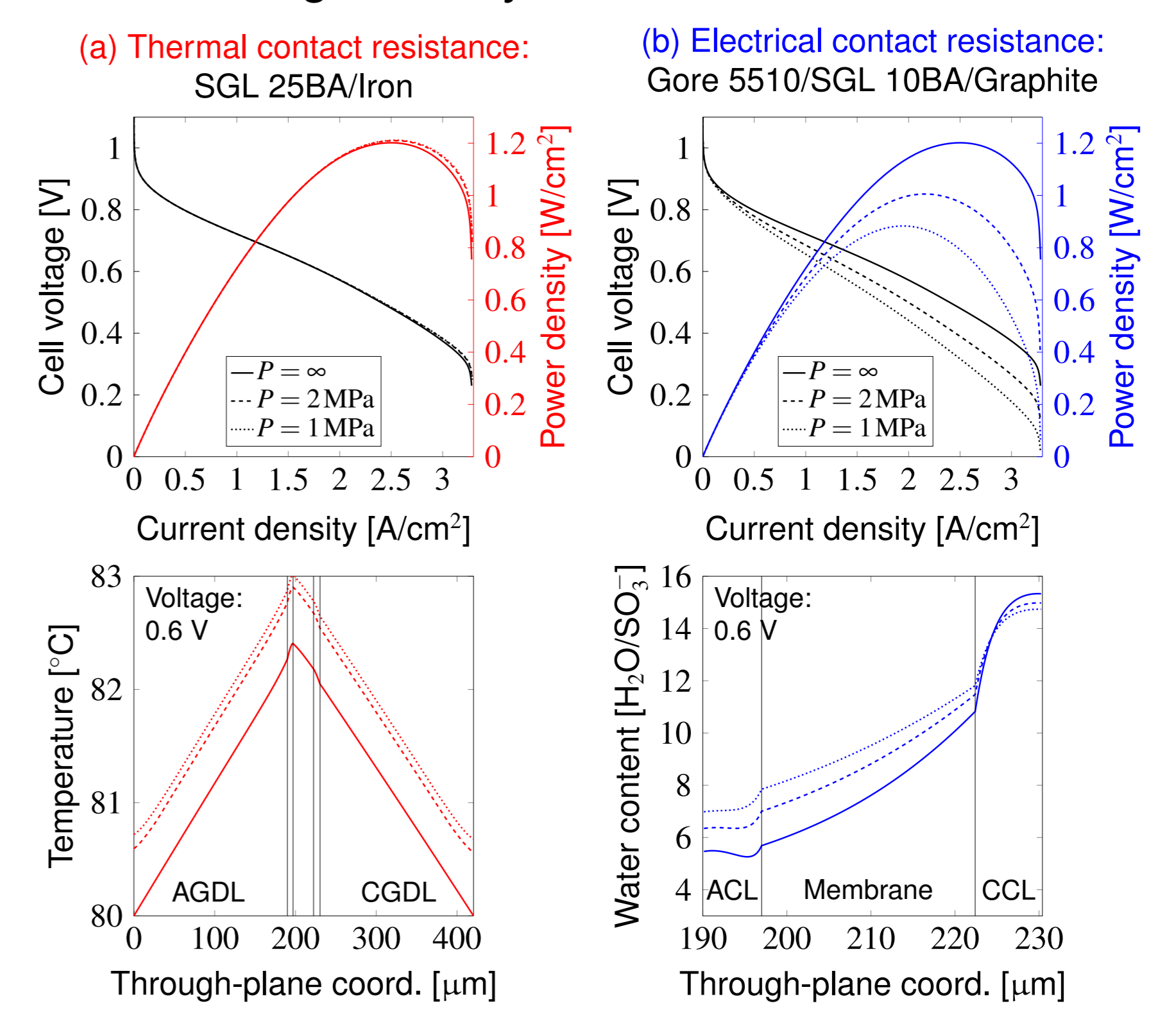


Fig. 4: Effect of contact resistance on fuel cell operation as computed with the 1D finite element model.

Conclusion

Our simulations demonstrate that (i) thermal contact resistance leads to a moderate temperature increase within the PEFC, (ii) electrical contact resistance is responsible for a significant voltage loss even at high clamping pressures, and that (iii) this performance drop increases with current density, as shown in Fig. 4. These results challenge researchers in PEFC modeling not to neglect interfacial resistance in their computational studies. Contact resistance constitutes an important step toward more predictive fuel cell models.

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