Introduction: Two complementary 3D models were coupled to the overall modeling of PEM fuel cell. The modeling required multiphysics processes: gas flow at the distribution channels and porous media flow at GDL (model 1 – Entire Plate model); electrochemical reactions at catalyst layer and ionic charge transport at membrane (model 2 – MEA model). A schematic view of the regions where those phenomena occur is presented in Figure 1.

Computational Methods:
Five reference channels were chosen to represent the Entire Plate model (Figure 2). These channels allow sampling of pressure and it was tabulated as initial values in MEA model (Figure 3). In the first model, Free and Porous Media Flow and Brinkman Equations were implemented in the flow channels and the GDL, as:

$$\frac{\partial \rho}{\partial t} - \nabla \cdot (\rho \mathbf{u}) + \rho \mathbf{u} \cdot \nabla \mathbf{u} + \nabla p = 0$$

$$\mathbf{V} \cdot \mathbf{u} = 0$$

$$\rho \frac{\partial \mathbf{u}}{\partial t} - \nabla \cdot (\mathbf{D} \nabla \mathbf{u}) = \nabla \cdot \mathbf{F} + \mathbf{S}$$

where $\mathbf{u}$ is the velocity vector, $\rho$ is the fluid density, $p$ is the pressure, $\mathbf{F}$ is the force vector, and $\mathbf{S}$ is the source vector. The Laplace equation for the potential $\phi$ is:

$$\nabla^2 \phi = 0$$

Boundary conditions (B.C.) for the Laplace equation include:

- $\mathbf{n} \cdot \mathbf{u} = 0$ on the boundary of the fuel cell
- $\mathbf{n} \cdot \mathbf{v} = 0$ on the boundary of the fuel cell

Mathematical coupling of models (Figure 4):

Results: Numerical results of anode and cathode mass fractions, current density, pressure, velocity and convergence graphics were generated in the COMSOL Multiphysics® software. The polarization planes generated from MEA model are showed in Figure 5, highlighting the potential dependence of current density at cathode collector. These readings were obtained from the interface electrode-membrane, at T=348K (75°C), pref=1 atm, pH$_{H_2}$=pO$_2$= 52.45 Pa, 0<E(V)<1.0. In Figure 6 one can observe the non-uniform distributions of ionic current density in the middle plane of the membrane.

Conclusions: The strategy of coupling two 3D models satisfy the requirements of the comprehensive model of a unitary Proton Exchange Membrane fuel cell, including its internal geometries and constitutive materials, as well as distinct physical and chemical processes was successfully performed. The final model is robust and useful as a tool for design and optimization of PEM fuel cells in a wide range of operating conditions.

Acknowledgments:

References: