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2 D dependence of Dimensionless Equations in Hydrogen/Oxygen Polymer Electrolyte Fuel Cells; Smooth Platinum Electrodes.

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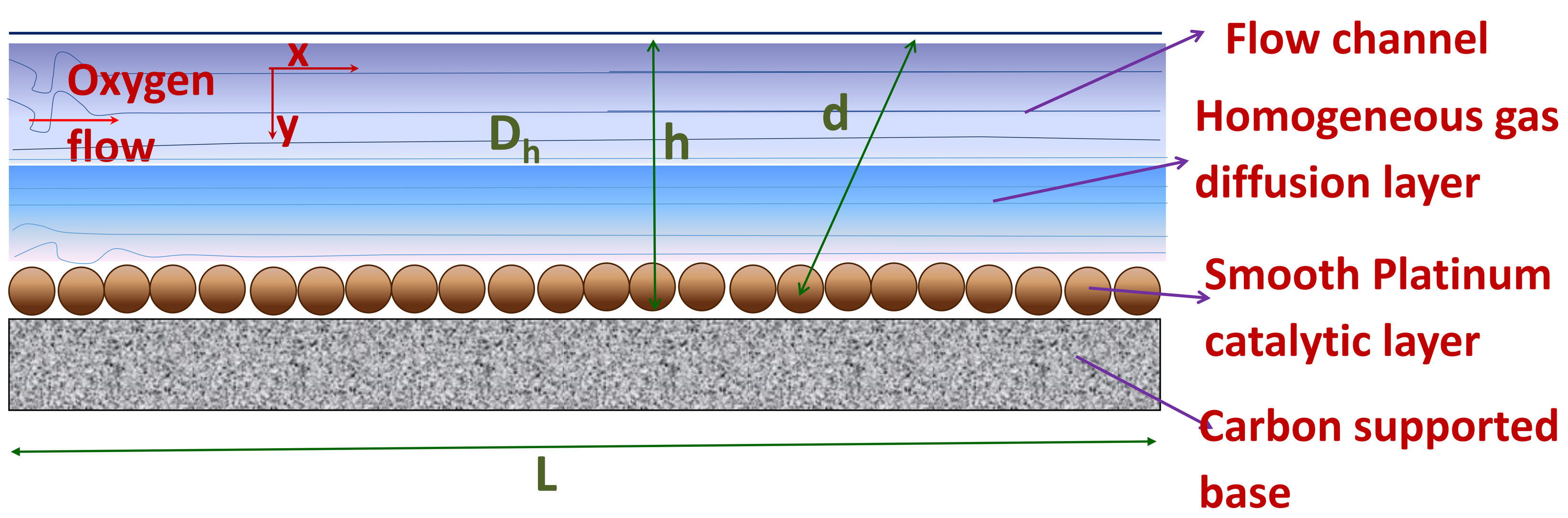
Summary

One of the problems in the optimization of a fuel cell performance is the operation prediction without much time of computations. The employ of exact analytical functions for picturing the distribution of potential and current densities in 2D PEMFCs generalizes the study and reduces large numeric or iteration times for each experimental situation. Therefore, we foresee analytical solutions for mass balance equations using the asymptotic velocity equations (normal and tangential coordinates) to obtain 2D concentration, current and overpotential profiles for smooth platinum catalysts. Dimensionless numbers are deduced, *i.e.* Wagner, Damkoehler and Graetz to characterize the fuel cell performance, first with a 1D approach and also along 2D coordinates. Besides, the complete polarization curve is predicted comparing the theoretical results with the proper variations of electrochemical magnitudes in a single home-made hydrogen/oxygen 200 cm² PEMFC.



Scheme 1.- Oxygen flow stream along the cathodic channel of a 2D fuel cell. Thin catalytic layer of smooth platinum ensembles at a steady state laminar linear semi-infinite flow.

Polarization Curves

$$j(\xi) = \frac{4nFU^{o3/2}}{\sqrt{\nu}}\left(-\frac{\left[4\frac{U^{o3/2}}{D\sqrt{\nu}}+1\right]}{\frac{2U^{o3/2}}{D\sqrt{\nu}}+8\xi^2+4\xi+2} - \frac{2\xi+1}{8\left[4\frac{U^{o3/2}}{D\sqrt{\nu}}+4\xi^2+2\xi+1\right]} + \frac{1}{4} \right)$$

$$\exp\left\{ \frac{U^{o3/2}}{4D\sqrt{\nu}}\left(-\log\left(4\frac{U^{o3/2}}{D\sqrt{\nu}}+4\xi^2+2\xi+1\right) - \frac{8\left(\frac{4U^{o3/2}}{D\sqrt{\nu}}+1\right)}{\sqrt{4\frac{U^{o3/2}}{D\sqrt{\nu}}+3}}\tan^{-1}\left(\frac{4\xi+1}{\sqrt{4\frac{U^{o3/2}}{D\sqrt{\nu}}+3}}\right) + 4\xi \right)\right\}$$

$$\eta(\xi) = b\ln\left(\frac{j_o}{C^o}\right) - b\ln\left(\frac{nF\left(\frac{U^o 2\sqrt{2}}{\sqrt{\nu}}\right)\xi^2}{2\frac{U^o}{D}+4\xi^2+2\xi+1}\right)$$

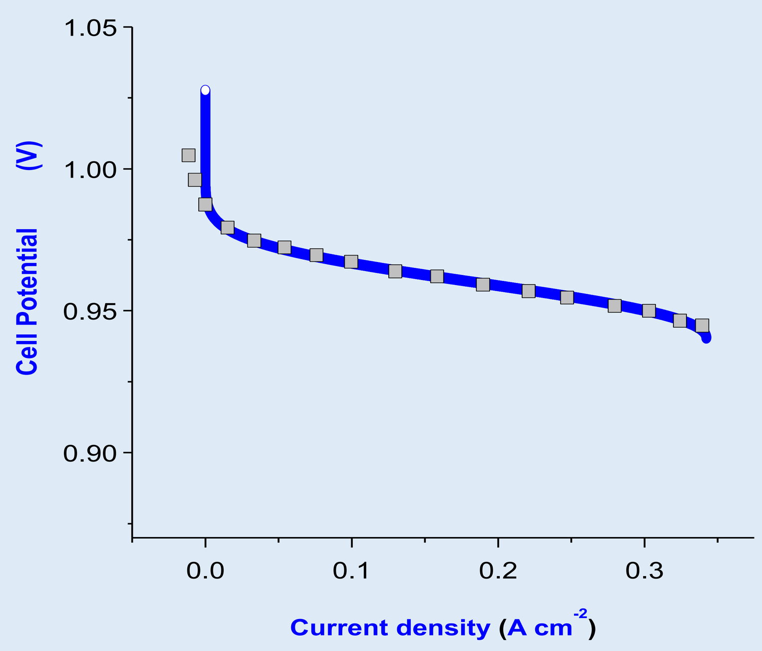


Figure 2.- Cell Potential vs. Current Density. ν=0.01 cm²s⁻¹, **U°** = 0.16 cm s⁻¹, **D** = 0.02 cm²s⁻¹. **C°**= 10⁻³ mol cm⁻³ **j$_o$** = 0.5 Acm⁻² **b**=0.03 V dec⁻¹, **n**=4

2 D Velocity Profile

$$v_x\left(\frac{\partial v_x}{\partial x}\right) + v_y\left(\frac{\partial v_x}{\partial y}\right) = \nu\left(\frac{\partial^2 v_x}{\partial y^2}\right) + \nu\left(\frac{\partial^2 v_x}{\partial x^2}\right)$$

Dimensionless velocity $v_x^* \equiv \frac{v_x}{U^o}$

From the Continuity Equation : $v_y = -\int \frac{\partial v_x}{\partial x}dy$ with $v_{y=0} \equiv 0$

Similarity Mechanics $\xi \equiv \frac{y}{2\sqrt{x}}\sqrt{\frac{U^o}{\nu}}$

Cauchy-Euler Equation:

$$\frac{2\,cte}{U^o}\xi\left(\frac{dv_x^*}{d\xi}\right) + \left(\frac{d^2 v_x^*}{d\xi^2}\right) = 0$$

$v_x^*(x=0)=0$, $v_x^{*'}(x=0)=1$

$$v_x(x,y) = U^o\,\mathrm{erf}\left(\sqrt{\frac{\pi U^o}{16\nu}}\frac{y}{\sqrt{x}}\right)$$

Continuity Equation →

$$v_y(x,y) = -\frac{2\sqrt{U^o\nu}}{\pi\sqrt{x}}\exp\left(-\frac{\pi U^o}{16\nu}\frac{y^2}{x}\right)$$

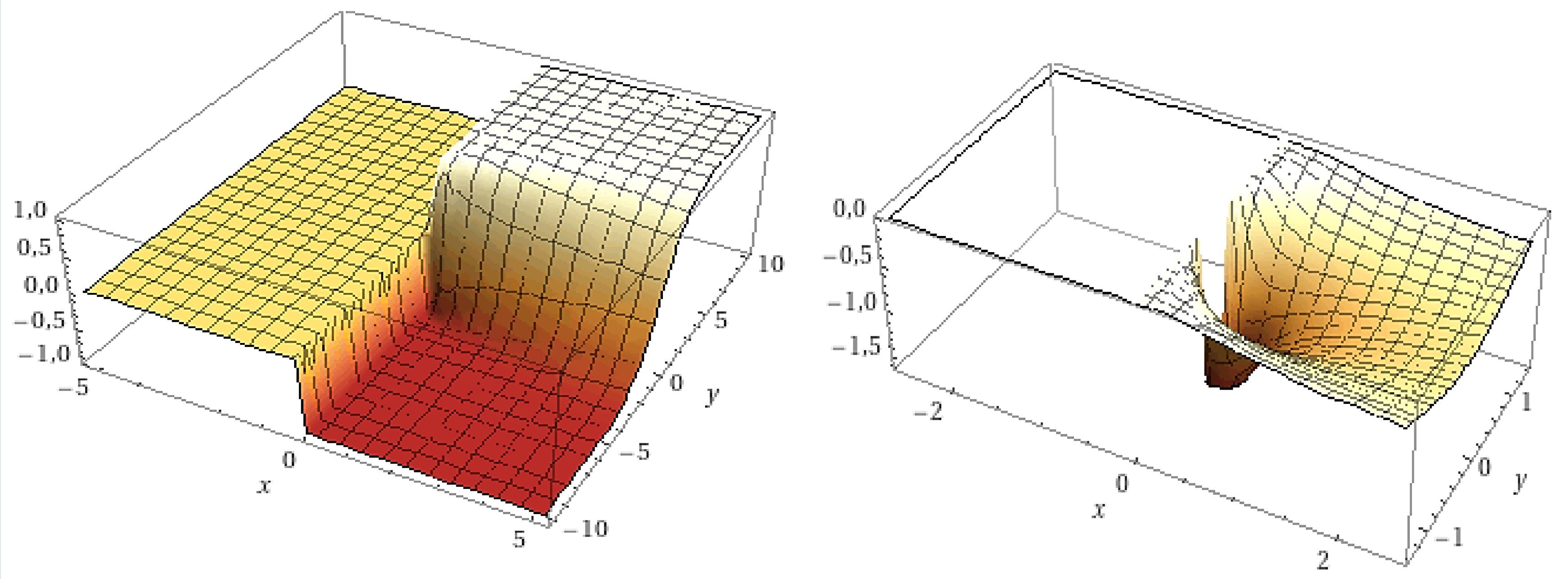
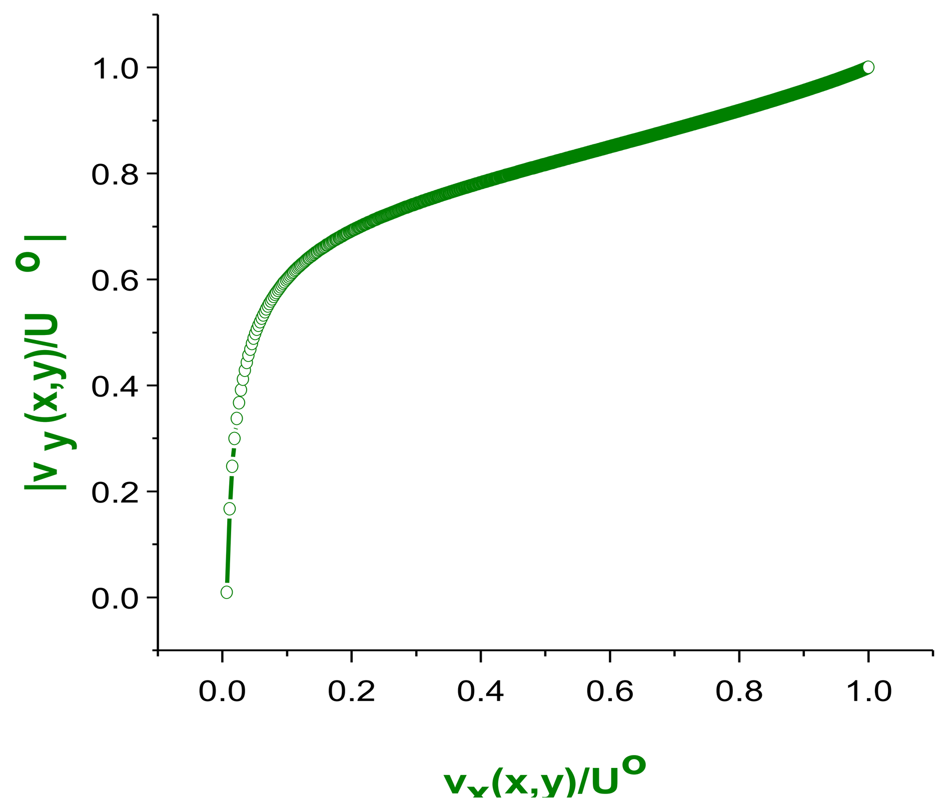


Figure 1.- Real Part 3D plot of **v$_x$(x,y)** (left panel) and **v$_y$(x,y)** (right panel). **Lower Panel** asymptotic velocity solutions.



Asymptotic solutions

$$v_x(x,y)_{y\to 0} = \frac{U^{o3/2}y}{5.2\nu^{1/2}x^{1/2}}$$

$$v_y(x,y)_{y\to 0} = \frac{U^{o3/2}y^2}{140.6\nu^{1/2}x^{3/2}}$$

Dimensionless Numbers

The Wagner (**Wa**), Damkoehler (**Da**), Schmidt (**Sc**) and Graetz (**Gz**) numbers define the electrochemical reactor dimensionless equation:

$$Da_i = \frac{j_{o,c}d}{nFDC^o} \qquad w \equiv \frac{\sqrt{L}(2h-D_h)}{h\sqrt{D_h}}$$

$$Da = \frac{3Da_i Sc^{1/6}}{Gz^{1/2}}w\sqrt{X}e^{-N(X)}e^{-J(Y)/Wa} \qquad Da = \frac{3Da_i Sc^{1/6}w}{WaGz_{xy}^{1/2}}$$

Being **Da$_i$** the onset Damkoehler number and **w** the characteristic length on the PEMFC. **N(X)** and **J(Y)** are the overpotential and current distributions.

$$Da = \frac{j_o e^{-\alpha f(E-E_{j=0})}}{nFDC^o/\delta} \qquad Wa = \frac{b/j_o}{R_\Omega} \qquad Gz = \frac{D_h}{L}\mathrm{Re}\;Sc$$

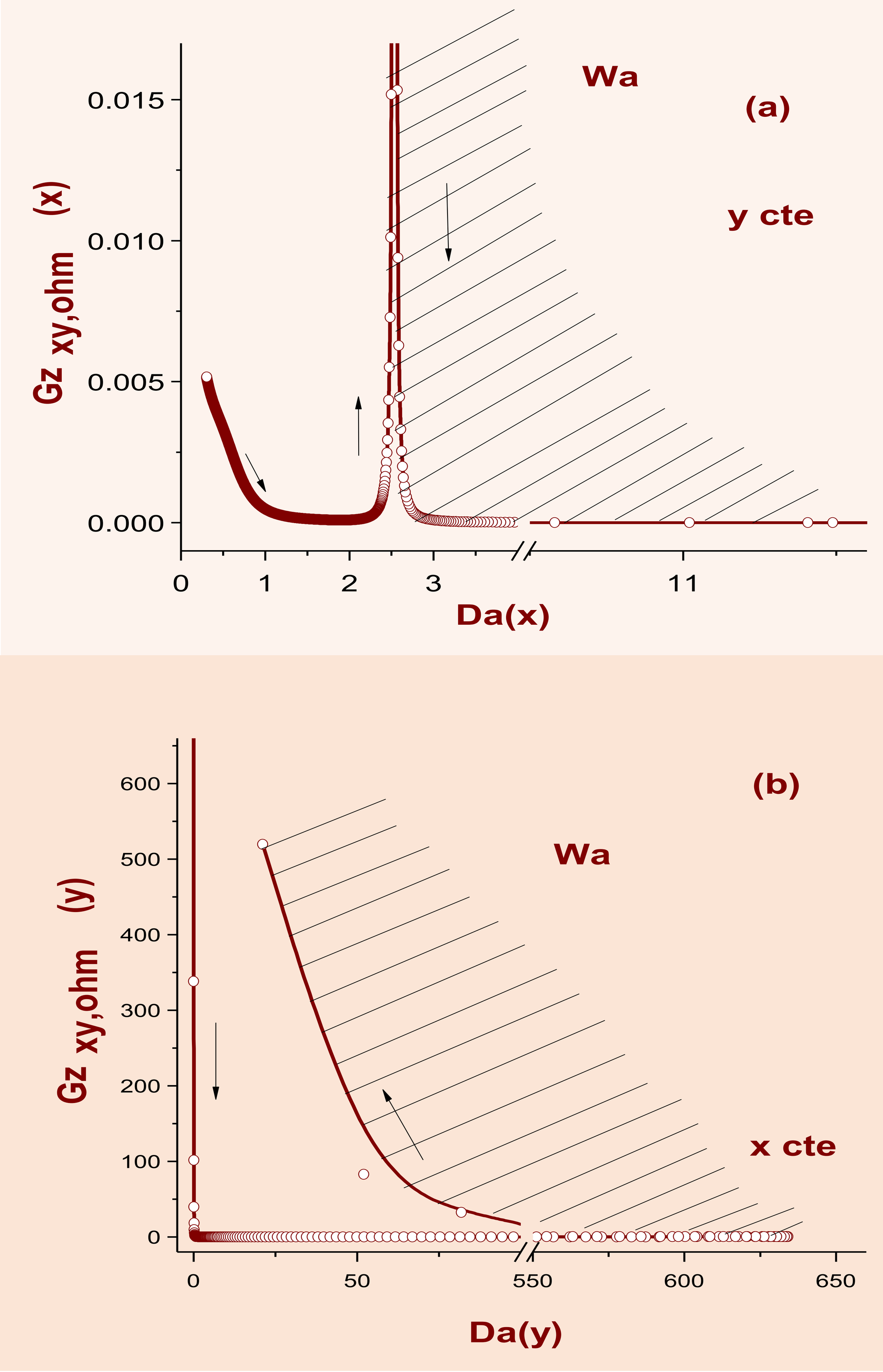


Figure 3.- Local bidimensional **Gz$_{xy}$** number as a function of **Da(x)**, Upper Panel **(a)**, and as a function of **Da(y)**, Lower Panel; **(b)** for the PEMFC with smooth surfaces.

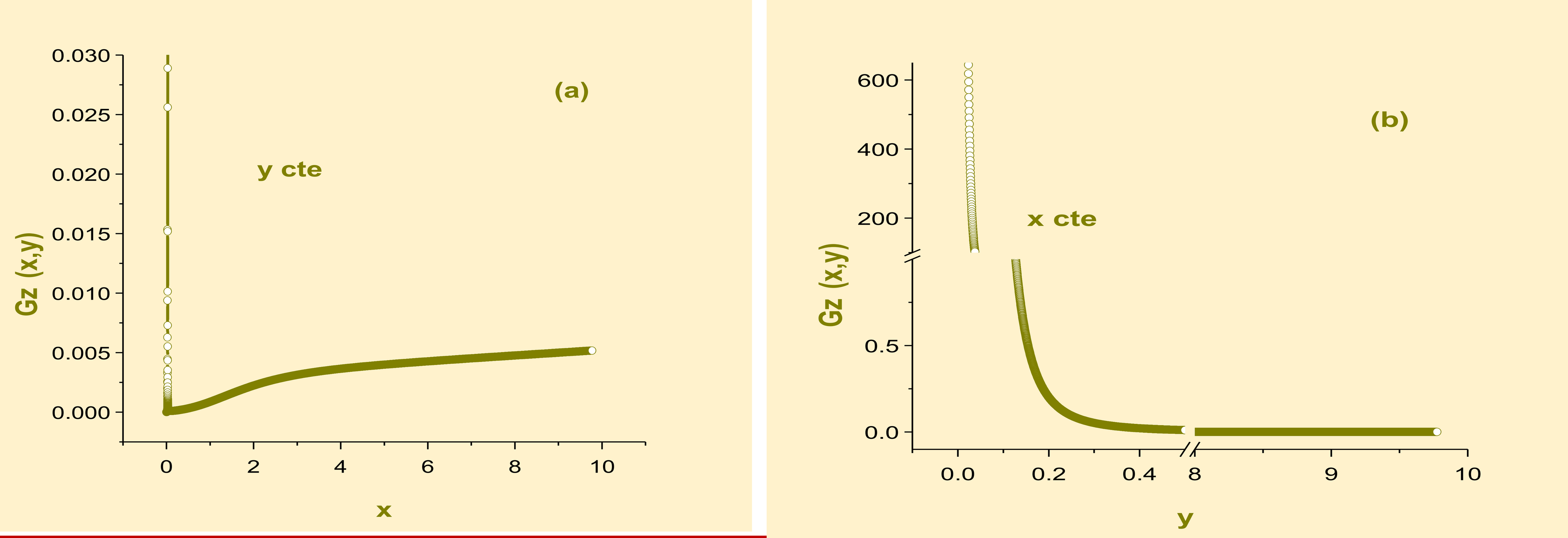


Figure 4.- Local bidimensional **Gz$_{xy}$** number under 2 D conditions as a function of **x (a,** left panel**)** and **y (b,** right panel**)** for the PEMFC with smooth surfaces.