

Optimal shape design and hydrogen fuel cells

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Today main energy sources

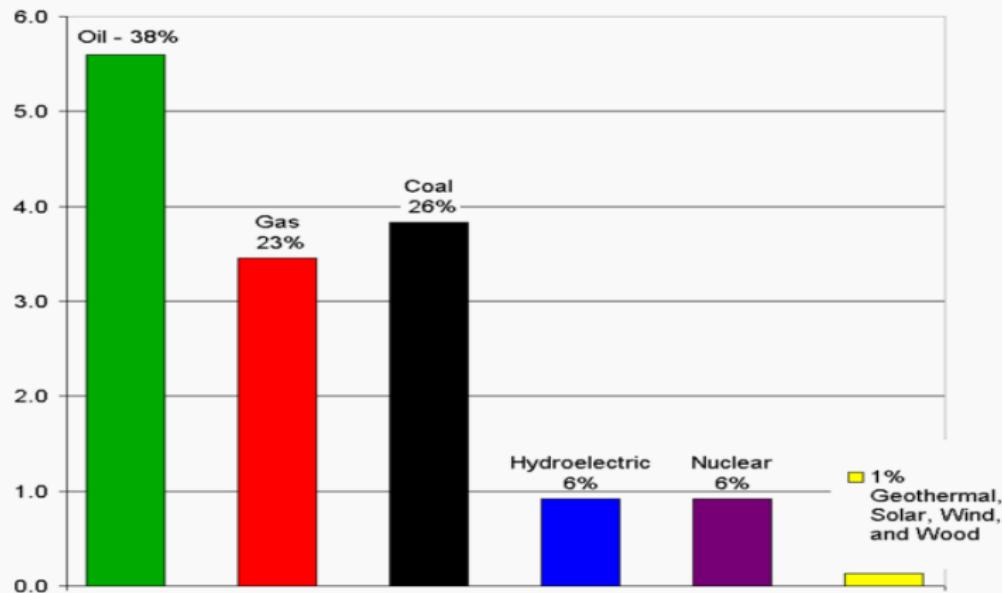
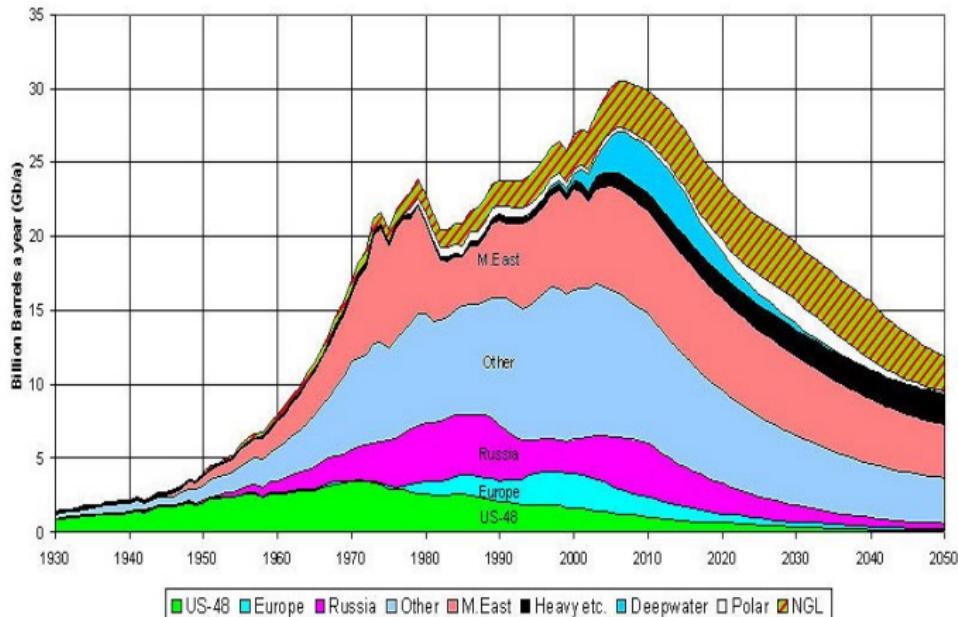


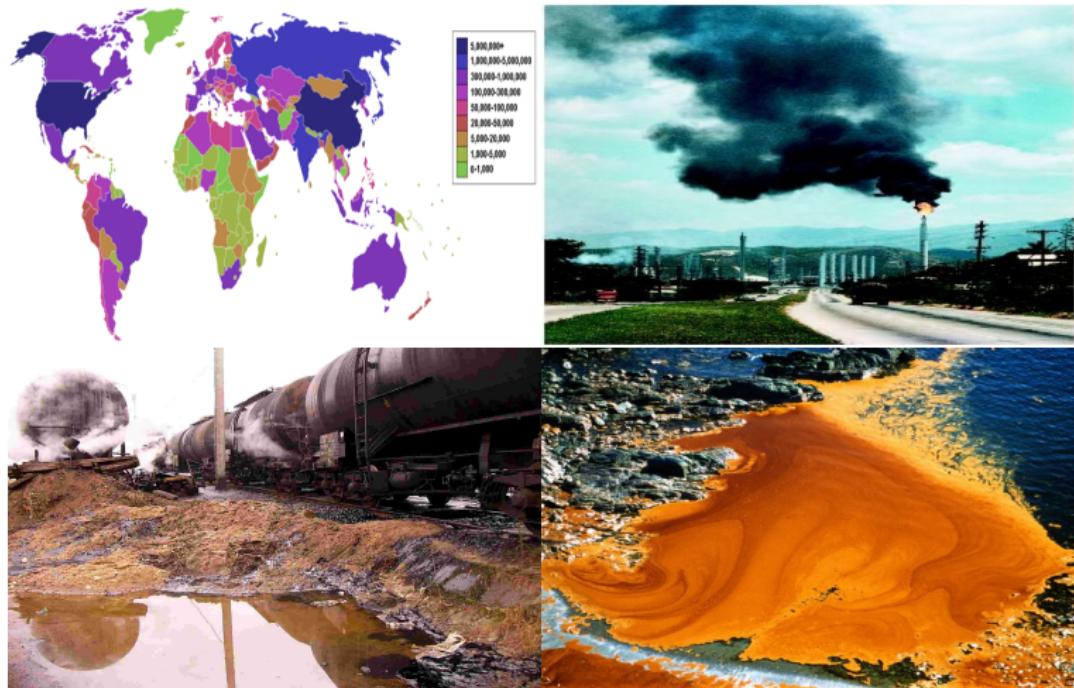
Figure: World main energy sources (in $TW=10^{12} W$)

... how much oil remains?

- It is thought that the peak oil will be reached **before 2020**

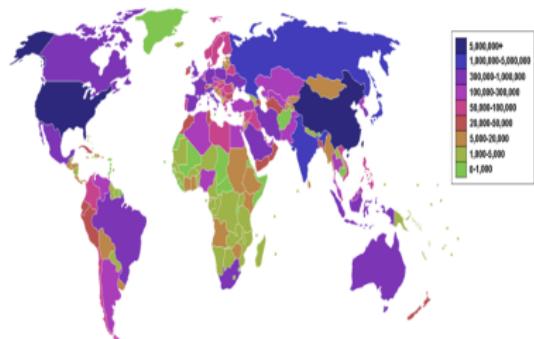


... and some consequenses



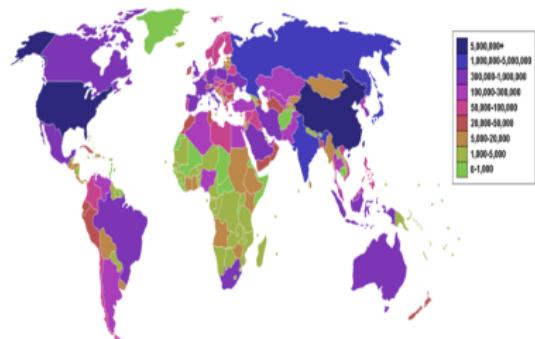
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- Global warming (carbon dioxide emissions)

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What are the alternatives?

- Renewable energy

- Wind power
- Hydropower
- Solar energy
- Biomass
- Biofuel
- Geothermal energy
- Nuclear energy (?)

- Hydrogen energy

Produces clean energy (electric current and water)

Issues:

- Production of hydrogen
- Storing and transporting hydrogen
- Extracting energy from hydrogen: **proton exchange membrane hydrogen fuel cells (PEM HFC)**

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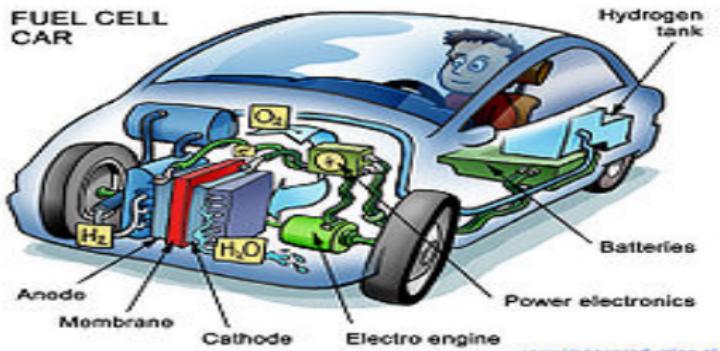
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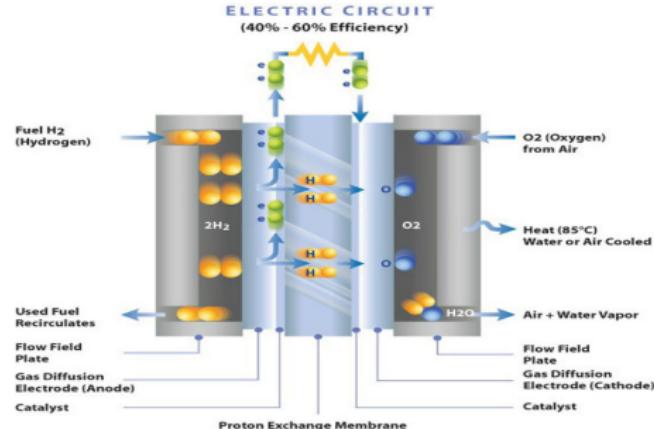
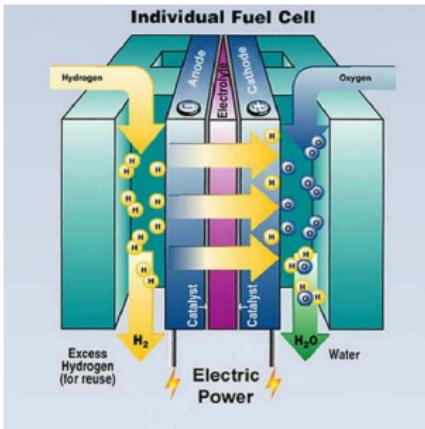
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Several car manufacturers in PEM HFC race



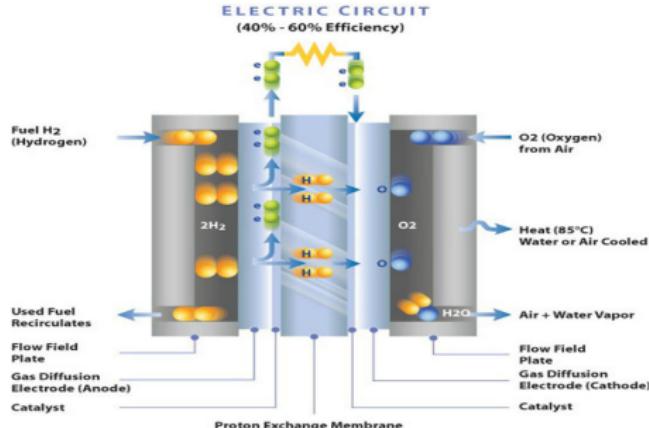
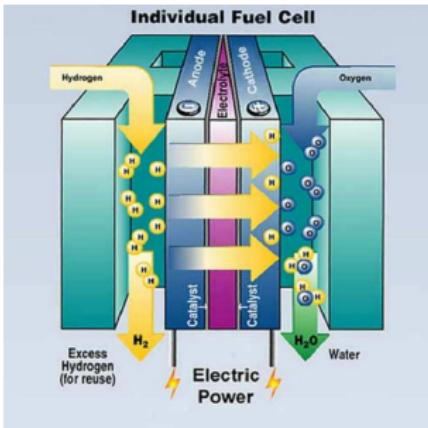
What is a PEM HFC, how it works?



How the energy is produced?

- At the anode: $2\text{H}_2 = 4\text{H}^+ + 4\text{e}^-$
- At the cathode: $\text{O}_2 + 2\text{e}^- = 2\text{O}^-$
- At the catalyst layer: $4\text{H}^+ + 2\text{O}^- = 2\text{H}_2\text{O}$

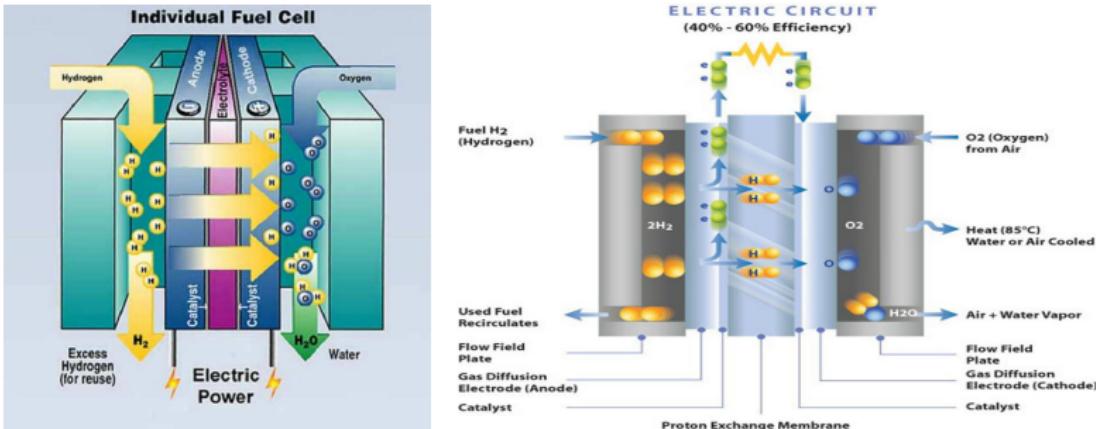
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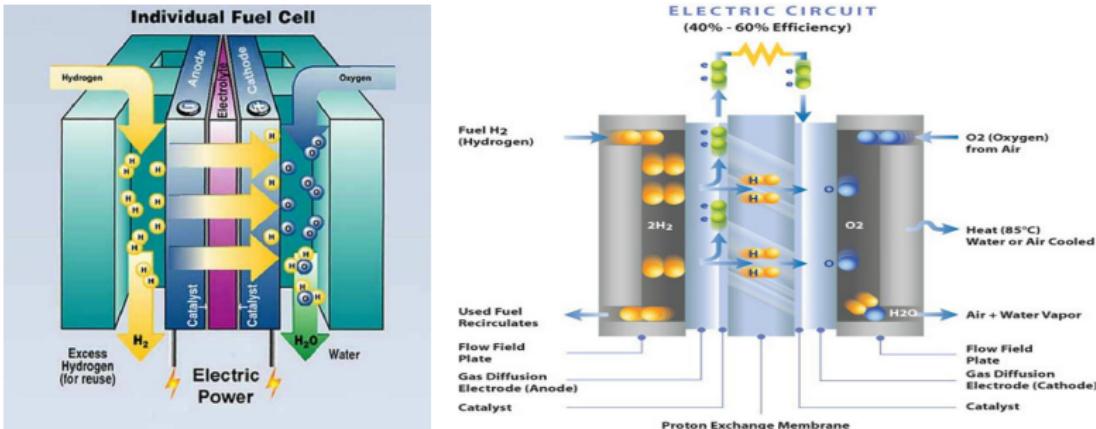
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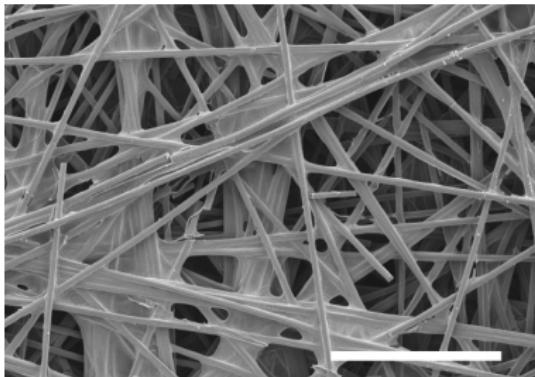
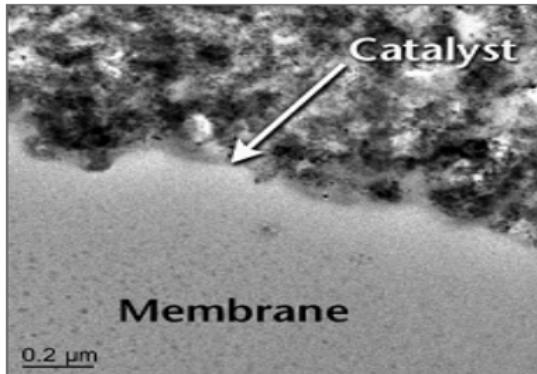
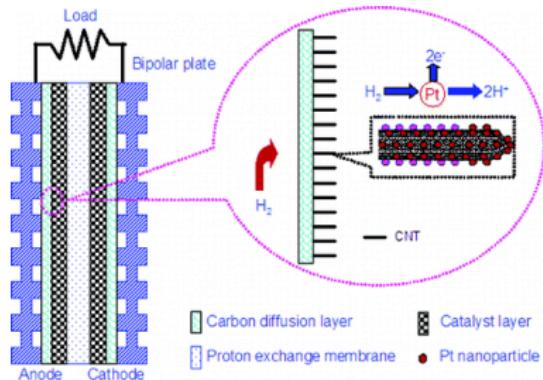
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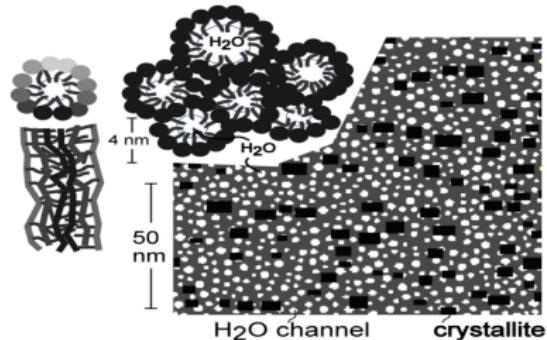
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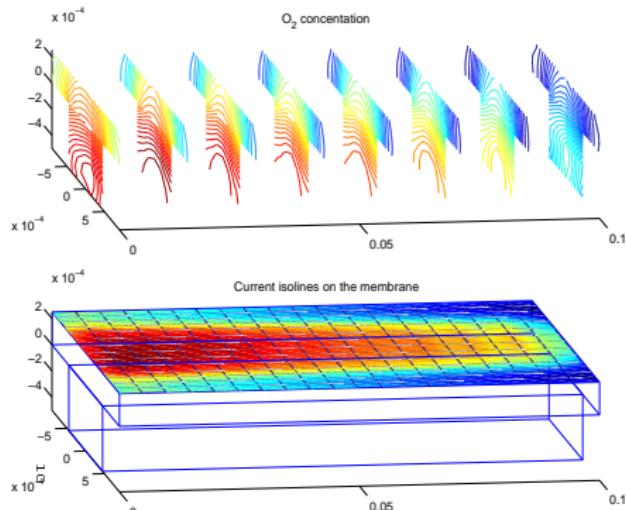
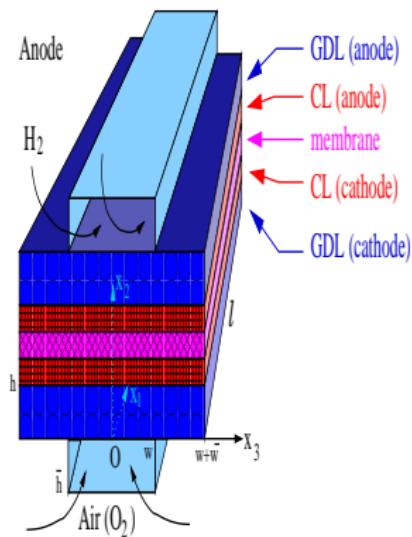


Water Channel Model



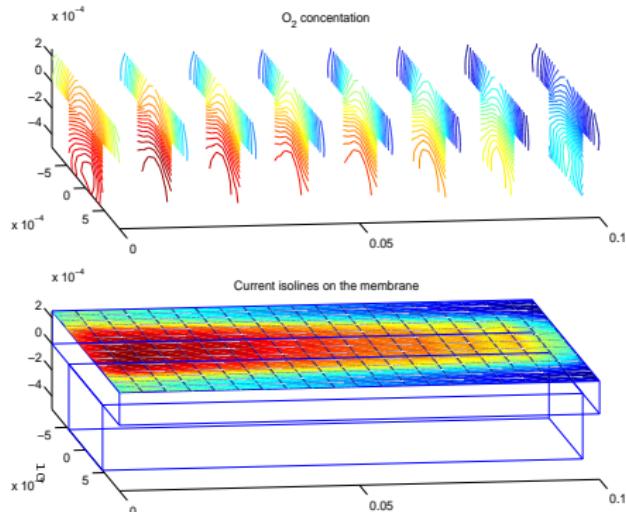
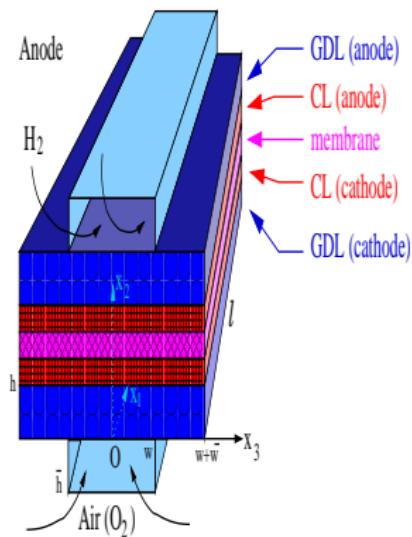
Inside PEM HFC: numerical computations

- Dry model, cathode channel and GDL, only one cell
- Variables:
 C_{O_2} , C_{H_2O} , \mathbf{u} , p , T



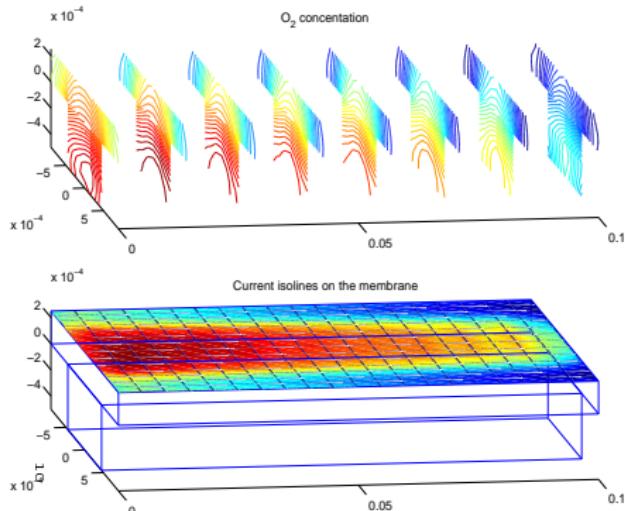
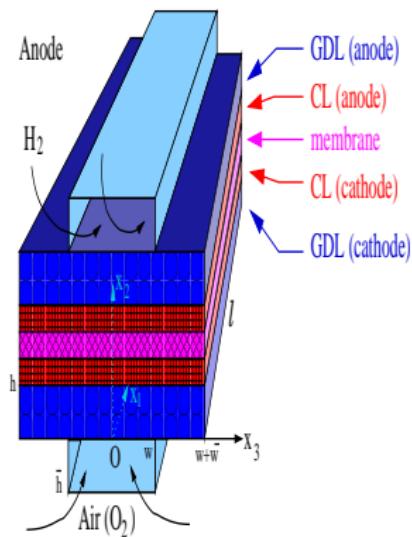
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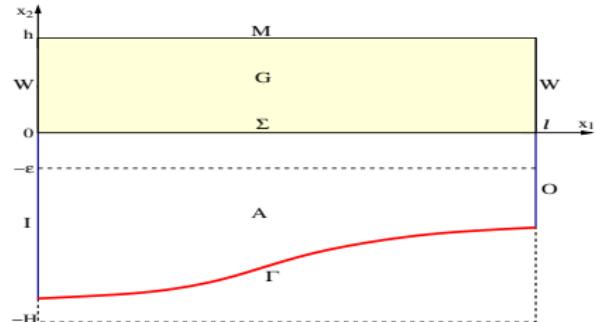
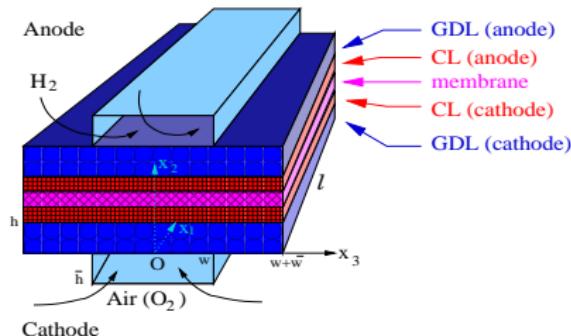


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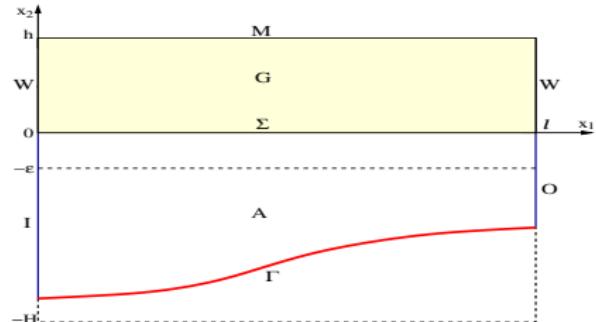
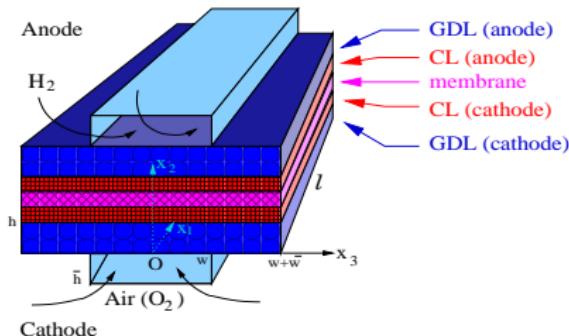


The model: geometry and variables



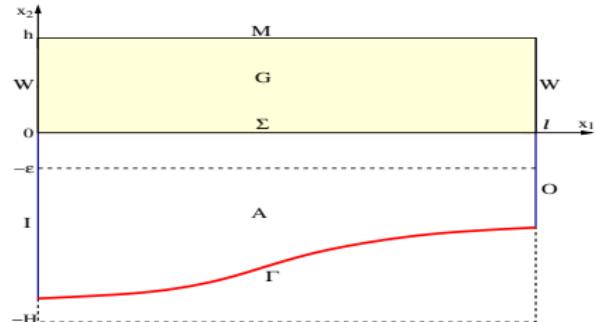
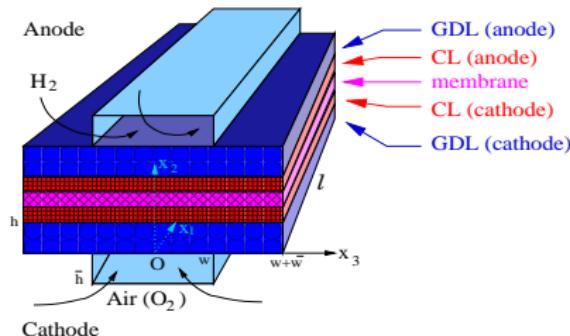
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- Variables:
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- Dimensions:
 $H=5 \cdot 10^{-2}$ m, $\epsilon=10^{-3}$ m, $h=3 \cdot 10^{-3}$ m, $\ell=0.4$ m

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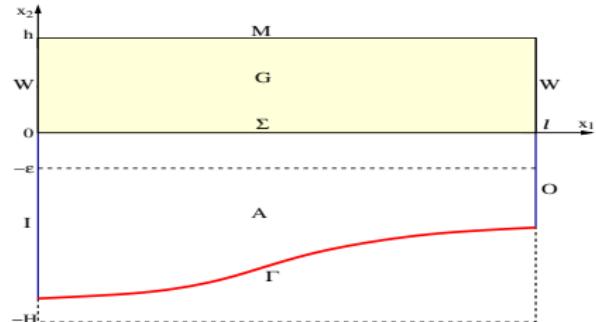
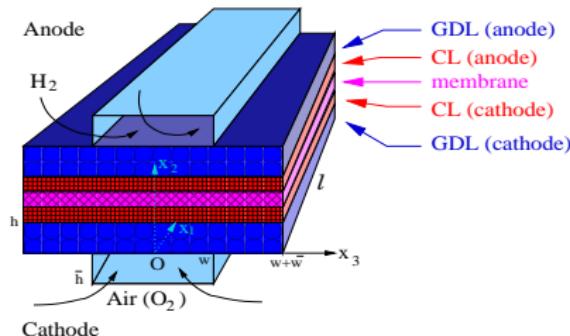
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The model: the equations

• The equations

$$A(\mathbf{u}) + B(p) := (-\mu \Delta \mathbf{u} + \nabla p) \chi_A + \left(\frac{\mu}{K} \mathbf{u} + \nabla p \right) \chi_G = 0 \quad \text{in } \Omega$$

$$B^t(p) := \nabla \cdot \mathbf{u} = 0 \quad \text{in } \Omega$$

$$C(c, \mathbf{u}) := -\mathcal{D} \Delta c + \mathbf{u} \cdot \nabla c = 0 \quad \text{in } \Omega,$$

• Boundary conditions

	c	\mathbf{u}	p
$I:$	$c = c_i$	$(\int_I u_1, u_2) = (\phi, 0)$	$p = p^i$
$O:$	$\partial_\nu c = 0$	$u_2 = 0$	$p = p^o$
$\Gamma:$	$\partial_\nu c = 0$	$(u_1, u_2) = (0, 0)$	
$\Sigma:$	$[c] = [\partial_2 c] = 0$	$(u_1(0^-), [u_2]) = (0, 0)$	$[p] = 0$
$W:$	$\partial_\nu c = 0$	$u_1 = 0$	
$M:$	$\mathcal{D} \partial_\nu c = -H_m c$	$u_2 = -z_m(c)$	

z_m smooth function, $z_m(c) = H_m \frac{c}{c_m + c}$ for $c \geq 0$.

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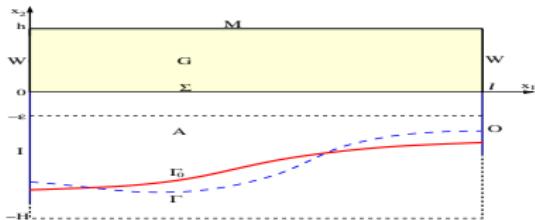
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The model: the objective

- The domain variation

$$\begin{aligned}\Theta &= C^2(\bar{\Omega}_0; \mathbb{R}^2) \\ &\cap \{\theta = (0, \theta_2), \theta_2 = 0 \text{ in } \{x_2 > -\epsilon\}, \\ &(\mathbb{I} + \theta)(\bar{\Omega}_0) \subset [0, l] \times [-H, h]\end{aligned}$$



- The set of **admissible shapes** is defined by

$$\mathcal{O} = \{\Omega_\theta = (\mathbb{I} + \theta)(\Omega_0), \theta \in \Theta\},$$

- The energy functionnal

$$E(\theta) = \frac{1}{2} w_u \left\| c - \int_M c \right\|_{L_2(M)}^2 - w_1 \int_M c - w_v \int_O c_v + w_p (p^i - p^o)$$

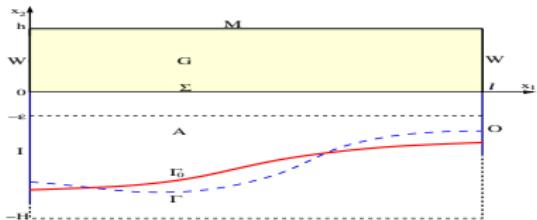
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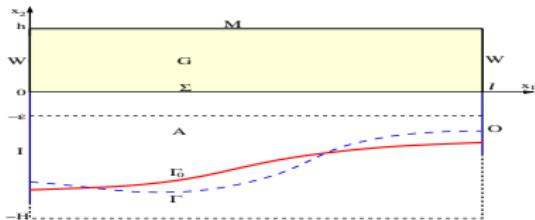
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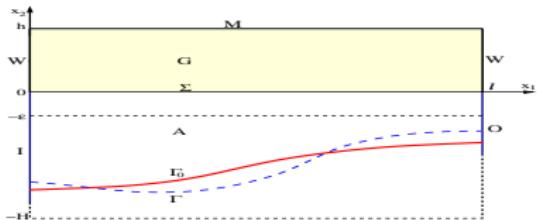
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Existence and uniqueness of state variables

Theorem 1

For any $\theta \in \Theta$, there exists a weak solution $(\mathbf{u}, \mathbf{p}, c)$ of

$$A(\mathbf{u}) + B(p) = 0, \quad B^t(\mathbf{u}) = 0, \quad C(c, \mathbf{u}) = 0,$$

subject to B.C. $D(\mathbf{u}, \mathbf{p}, c) = 0.$

If c^i is small enough then the solution is unique.

- Idea of the proof:

$$\begin{aligned}\alpha(\mathbf{u} + \mathbf{Z}(c), \mathbf{v}) + \beta(\mathbf{v}, \mathbf{p}) &= 0 \\ \beta(\mathbf{u}, \mathbf{q}) &= 0 \\ \gamma(c, \varphi; \mathbf{u} + \mathbf{Z}(c)) &= 0\end{aligned}$$

where

$$\beta(\mathbf{Z}(c), \cdot) = 0, \quad \mathbf{Z}(c) = -z_m(c) \text{ on } M.$$

Existence and uniqueness of state variables: idea

- There exists $\mathbf{Z} : H^1 \mapsto \mathbf{H}^1$, continuous and

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- Consider the operators T, S , $L = T \circ S$:

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$$c = S\hat{\mathbf{u}}, \quad \gamma(c, \varphi; \hat{\mathbf{u}}) = 0$$

- We have

T is continuous from H^1 to \mathbf{H}^1 , and compact in \mathbf{L}^r , $r > 2$

S is continuous from \mathbf{L}^r , $r > 2$ to H^1

- L has a fixed point $\hat{\mathbf{u}}$: $\hat{\mathbf{u}} = L\hat{\mathbf{u}}$ (unique if c^i small)

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Solution of shape optimization problem

Theorem 2

The problem:

$$\text{Find } \theta^* \in \Theta, \quad E(\theta^*) = \min\{E(\theta), \theta \in \Theta\}$$

has at least one solution in the class of uniform Lipschitz domains.

Idea of the proof:

- The set of uniform Lipschitz domains is compact
- The map

$$\theta \mapsto (\mathbf{u}_\theta, c_\theta)$$

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Shape differentiability of the energy

Theorem 3

Assume c^i is small enough. Then:

i) the map

$$\theta \mapsto (\mathbf{u} \circ (\mathbb{I} + \theta), \mathbf{p} \circ (\mathbb{I} + \theta), c \circ (\mathbb{I} + \theta))$$

is shape differentiable near $\theta = 0$ from Θ to $(\mathbf{U}_0, \mathbf{P}_0, C_0)$

ii) the energy functionnal $E(\theta)$ is differentiable and

$$\begin{aligned} E'(0)(\xi) &= \int_M (w_u(c - f_M c) - w_1) \partial_\theta c(\xi) \\ &+ w_v \int_O \partial_\theta c(\xi) \\ &+ w_p \partial_\theta p^i(\xi) \end{aligned}$$

Shape differentiability of the energy: idea of the proof (1)

- Find

$$(\mathbf{u}_\theta, \mathbf{p}_\theta, c_\theta) = (\mathbf{u} \circ (\mathbb{I} + \theta), \mathbf{p} \circ (\mathbb{I} + \theta), c \circ (\mathbb{I} + \theta)) \in \mathbf{U}_0 \times \mathbf{P}_0 \times C_0:$$

$$\alpha(\mathbf{u}_\theta + \mathbf{z}_\theta, \mathbf{v}; \theta) + \beta(\mathbf{v}, \mathbf{p}_\theta; \theta)$$

$$:= \int_{A_0} (\mu M_\theta \nabla (\mathbf{u}_\theta + \mathbf{z}_\theta) \cdot M_\theta \nabla \mathbf{v}) \text{Jac}(\mathbb{I} + \theta) + \int_G \frac{\mu}{K} (\mathbf{u}_\theta + \mathbf{z}_\theta) \cdot \mathbf{v}$$

$$- \int_{A_0} p_\theta \sum_{i,j=1}^2 M_\theta^{i,j} \partial_j \mathbf{v}_i \text{Jac}(\mathbb{I} + \theta) - p_\theta^i \int_{l_0} \mathbf{v}_1 (1 - \eta'(0)) = 0,$$

$$\begin{aligned} \beta(\mathbf{u}_\theta, q; \theta) &:= - \int_{A_0} q \sum_{i,j=1}^2 M_\theta^{i,j} \partial_j \mathbf{u}_{i,\theta} \text{Jac}(\mathbb{I} + \theta) - q^i \int_{l_0} \mathbf{u}_{1,\theta} (1 - \eta'(0)) \\ &= 0, \end{aligned}$$

$$\begin{aligned} \gamma(c_\theta, \varphi; \mathbf{u}_\theta + \mathbf{z}_\theta, \theta) &:= \int_{\Omega_0} (D M_\theta \nabla c_\theta \cdot M_\theta \nabla \varphi + \varphi (\mathbf{u}_\theta + \mathbf{z}_\theta) \cdot M_\theta \nabla c_\theta) \text{Jac}(\mathbb{I} + \theta) \\ &+ \int_M H_m c_\theta \varphi = - \int_M H_m \varphi \end{aligned}$$

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Shape differentiability of the energy: idea of the proof (2)

- Derivative at $\theta = 0$:

$$\alpha_0(\mathbf{u} + \mathbf{z}', \mathbf{v}) + \beta_0(\mathbf{v}, \mathbf{p})$$

$$\begin{aligned} &:= \int_{A_0} \mu \nabla(\mathbf{u} + \mathbf{z}') \cdot \nabla \mathbf{v} + \int_G \frac{\mu}{K} (\mathbf{u} + \mathbf{z}') \cdot \mathbf{v} - \int_{A_0} p \nabla \cdot \mathbf{v} - p^i \int_{l_0} \mathbf{v}_1 \\ &= l_1(\mathbf{v}), \end{aligned}$$

$$\beta_0(\mathbf{u}, q) := - \int_{A_0} q \nabla \cdot \mathbf{u} - q^i \int_{l_0} \mathbf{u}_1 = l_2(\mathbf{q}),$$

$$\gamma_0(c, \varphi, \mathbf{u}_0) + \int_{\Omega_0} (\mathbf{u} + \mathbf{z}') \cdot \nabla c_0 \varphi$$

$$\begin{aligned} &:= \int_{\Omega_0} D(\nabla c \cdot \nabla \varphi) + (\mathbf{u}_0 \cdot \nabla c) \varphi + \int_M H_m c \varphi + \int_{\Omega_0} \varphi (\mathbf{u} + \mathbf{z}'_0) \cdot \nabla c_0 \\ &= l_3(\varphi) \end{aligned}$$

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Shape differentiability of the energy: idea of the proof (3)

- We consider the operator T_0, S_0

$$\hat{\mathbf{u}} = S_0(c) = \mathbf{u} + \mathbf{z}'(c), \quad \alpha_0(\mathbf{u} + \mathbf{z}', \mathbf{v}) + \beta_0(\mathbf{v}, \mathbf{p}) = l_1(\mathbf{v}), \\ \beta_0(\mathbf{u}, \mathbf{q}) = l_2(\mathbf{q}),$$

$$c = S_0(\hat{\mathbf{u}}), \quad \gamma_0(c, \varphi; \mathbf{u}_0) + \int_{\Omega} (\hat{\mathbf{u}} \cdot \nabla c_0) \varphi = l_3(\varphi),$$

and $L_0 = T_0 \circ S_0 : \mathbb{L}^r \mapsto \mathbb{L}^r$

- L_0 is compact. If c^i is small L_0 has a unique fixed point.
- Implicit function theorem:

shape differentiability of $\theta \mapsto (\mathbf{u}_{\theta}, \mathbf{p}_{\theta}, c_{\theta})$

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Numerical computation of the optimal shape

- $E'(0)(\xi)$ involves

shape derivatives $\mathbf{u}', \mathbf{p}', c'$:

$$A(\mathbf{u}') + B(\mathbf{p}') = 0,$$

$$B^t(\mathbf{u}') = 0,$$

$$\partial_c C(c_0, \mathbf{u}_0) c' + \partial_{\mathbf{u}} C(c_0, \mathbf{u}_0) \mathbf{u}' = 0,$$

subject to B.C.

$$\partial_{\mathbf{u}} D(\mathbf{u}_0, \mathbf{p}_0, c_0) c' + \partial_{\mathbf{p}} D(\mathbf{u}_0, \mathbf{p}_0, c_0) \mathbf{p}' + \partial_v D(\mathbf{u}_0, \mathbf{p}_0, c_0) c' = 0.$$

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Adjoint variables

- Let $\mathbf{v} = (v_1, v_2)$, $\mathbf{q} = (q, q^i)$, σ , the adjoint variables:

$$(-\mu \Delta \mathbf{v} + \nabla q) \chi_{A_0} + \left(\frac{\mu}{K} \mathbf{v} + \nabla q \right) \chi_G + \sigma \nabla c_0 = 0 \quad \text{in } A_0 \cup G,$$

$$\nabla \cdot \mathbf{v} = 0 \quad \text{in } \Omega_0,$$

$$-D \Delta \sigma - \mathbf{u}_0 \cdot \nabla \sigma = 0 \quad \text{in } \Omega_0,$$

subject to

	σ	\mathbf{v}	\mathbf{q}
$I :$	$\sigma = 0$	$(\int_I v_1, v_2) = (\mathbf{w}_p, 0)$	$q = q^i$
$O :$	$D \partial_\nu \sigma + (\mathbf{u}_0 \cdot \nu) = \mathbf{w}_v$	$v_2 = 0$	$q = 0$
$\Gamma :$	$\partial_\nu \sigma = 0$	$(v_1, v_2) = (0, 0)$	
$\Sigma :$	$[\sigma] = [\partial_2 \sigma] = 0$	$(v_1(0^-), [v_2]) = (0, 0)$	$[q] = 0$
$W :$	$\partial_\nu \sigma = 0$	$v_1 = 0$	
$M :$	$D \partial_\nu \sigma + (H_m + \mathbf{u}_0 \cdot \nu) \sigma + q z'_m(c_0) = \mathbf{w}_m$	$v_2 = 0$	

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Adjoint variables and shape derivative of the energy

Theorem 4

Assume c^i is small enough.

Then the adjoint problem has a unique weak solution \mathbf{v} , \mathbf{q} , σ .
Furthermore, for all $\xi \in \Theta$ we have

$$E'(0)(\xi) = \int_{\Gamma_0} \left(\mu (\partial_\nu \mathbf{v}_0 \cdot \partial_\nu \mathbf{u}_0) - D(\partial_\nu \sigma_0 \cdot \partial c_0) \right) (\xi \cdot \nu)$$

Easy to compute

0. Fix Γ_0 .
1. Compute state variables, adjoint variables.
2. Compute E' .
3. Update the boundary: $\Gamma = (\mathbb{I} - \lambda E')(\Gamma_0)$.
4. If E' is small enough, stop.

Otherwise, set $\Gamma_0 = \Gamma$ and repeat steps 1-4.

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Numerical computations

- Remember E :

$$E(\theta) = \frac{1}{2} w_u \left\| c - \int_M c \right\|_{L_2(M)}^2 - w_1 \int_M c - w_v \int_O c_v + w_p (p^i - p^o),$$

where $c_v = 1 - c_n - c$, and c_n constant.

- Several choices of parameters w_u, w_1, w_v, w_p .

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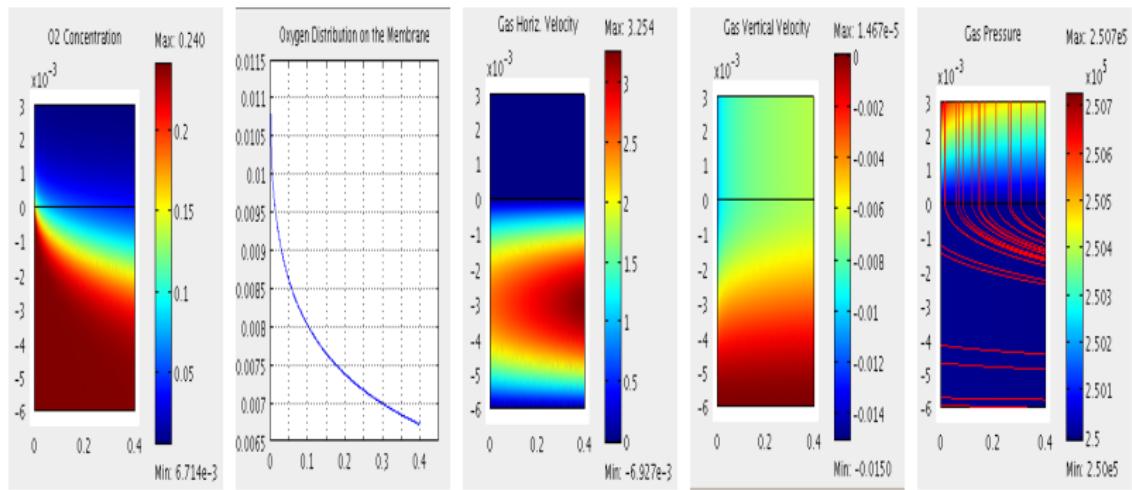
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Numerical computations: reference case

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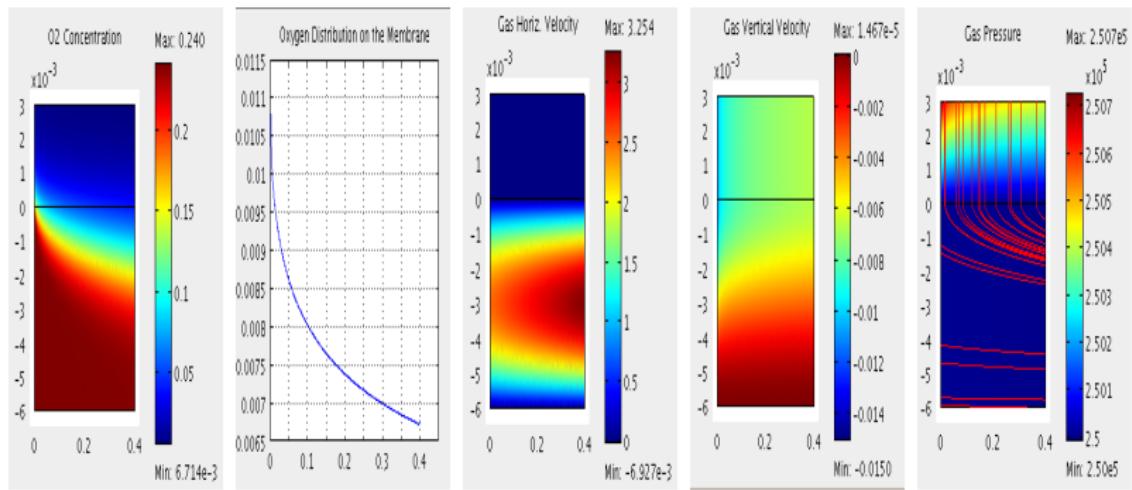
$$\begin{aligned}\ell &= 0.4[m], & h &= 3 \cdot 10^{-3}[m], & H_0 &= 6 \cdot 10^{-3} \\ \Gamma_0 &= [0, \ell] \times \{-H_0\}, & H &= 1 \cdot 10^{-2}[m], & \epsilon &= 1 \cdot 10^{-3}[m] \\ c^i &= 0.24, & c_n &= 0.75, & c_m &= 3.5 \\ \phi &= 0.005 [m/s], & p^o &= 250\,000 [Pa]\end{aligned}$$



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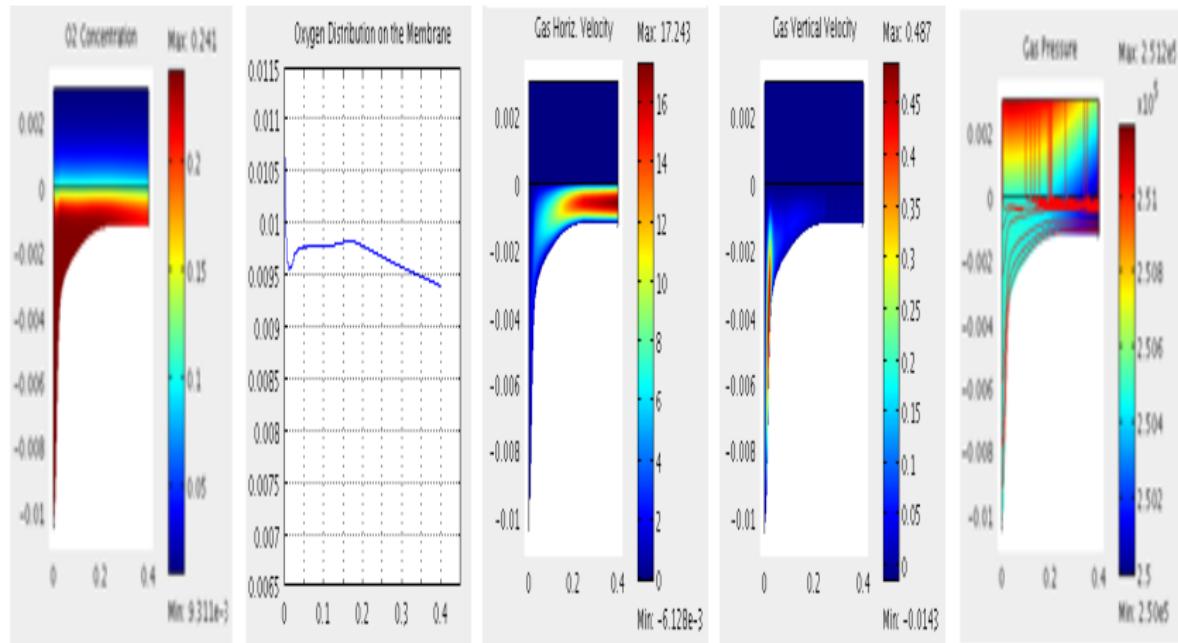
- Data:

$$\begin{aligned}\ell &= 0.4[m], & h &= 3 \cdot 10^{-3}[m], & H_0 &= 6 \cdot 10^{-3} \\ \Gamma_0 &= [0, \ell] \times \{-H_0\}, & H &= 1 \cdot 10^{-2}[m], & \epsilon &= 1 \cdot 10^{-3}[m] \\ c^i &= 0.24, & c_n &= 0.75, & c_m &= 3.5 \\ \phi &= 0.005 [m/s], & p^o &= 250\,000 [Pa]\end{aligned}$$



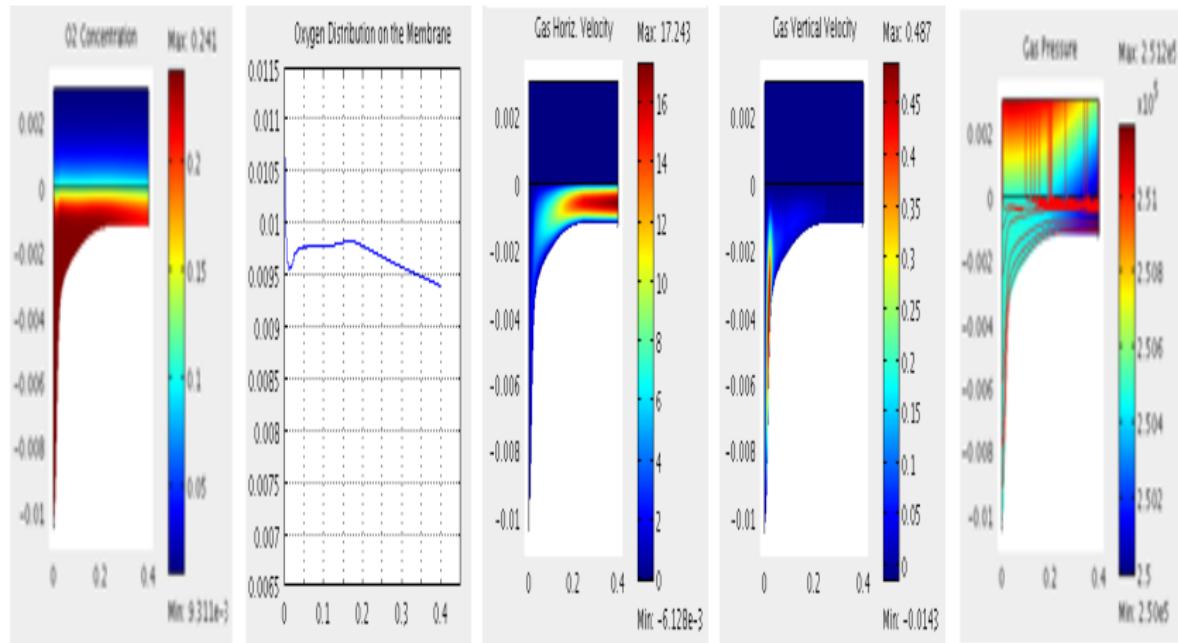
Numerical computations: w_u

- $w_u = 1, w_1 = w_v = w_p = 0$



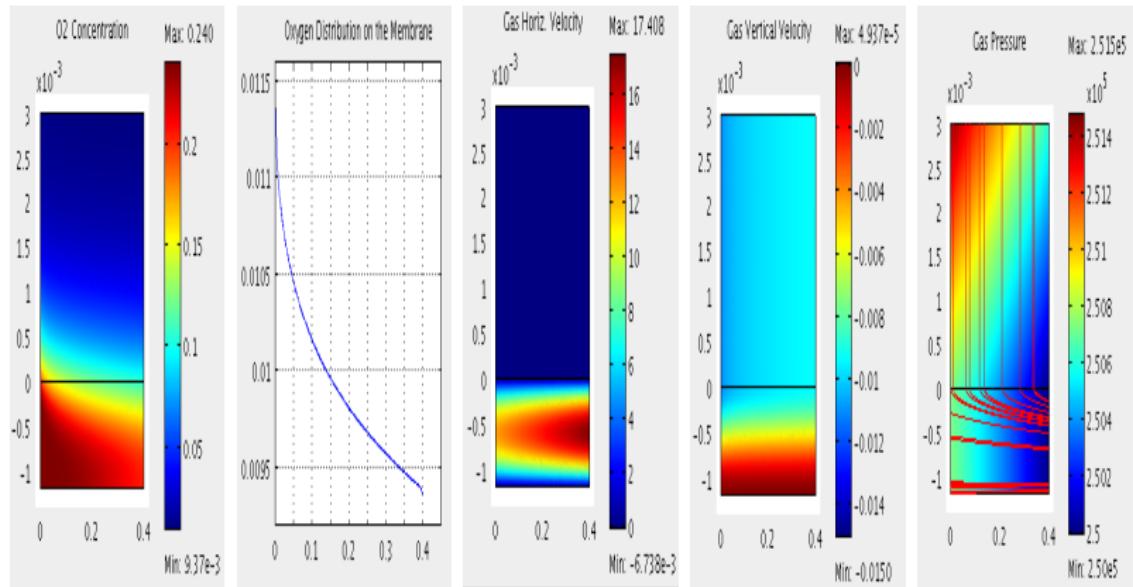
Numerical computations: w_u

- $w_u = 1, w_1 = w_v = w_p = 0$



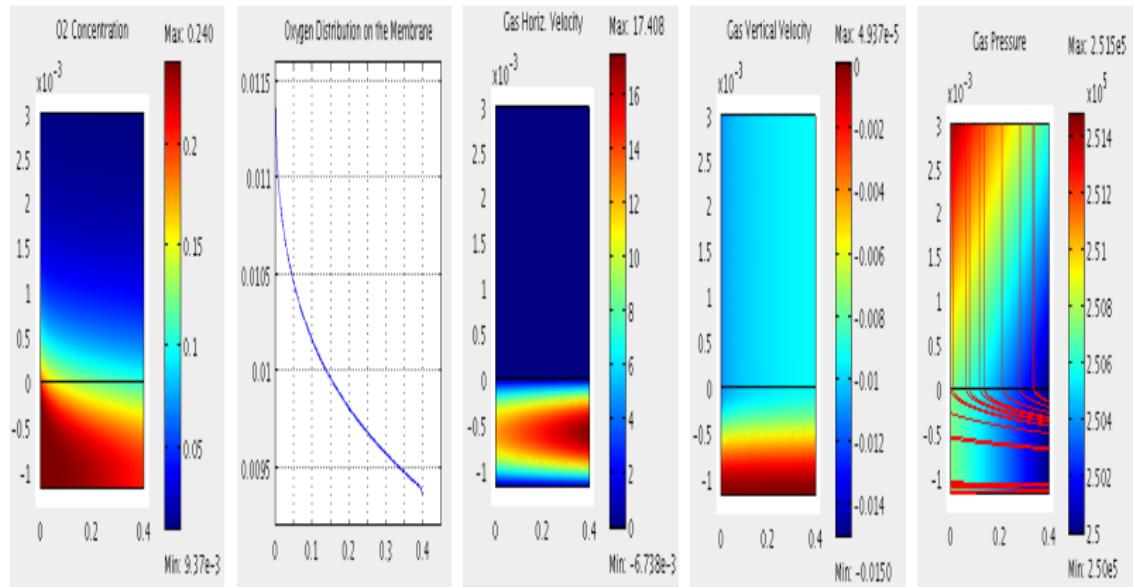
Numerical computations: w_1

- $w_u = 0, w_1 = 1, w_v = w_p = 0$



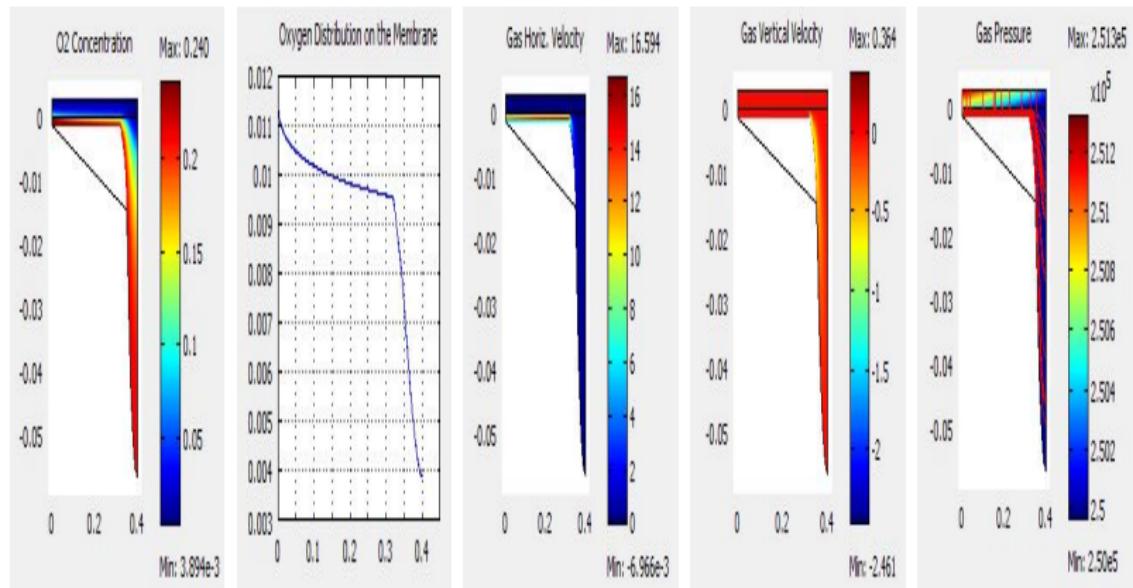
Numerical computations: w_1

- $w_u = 0, w_1 = 1, w_v = w_p = 0$



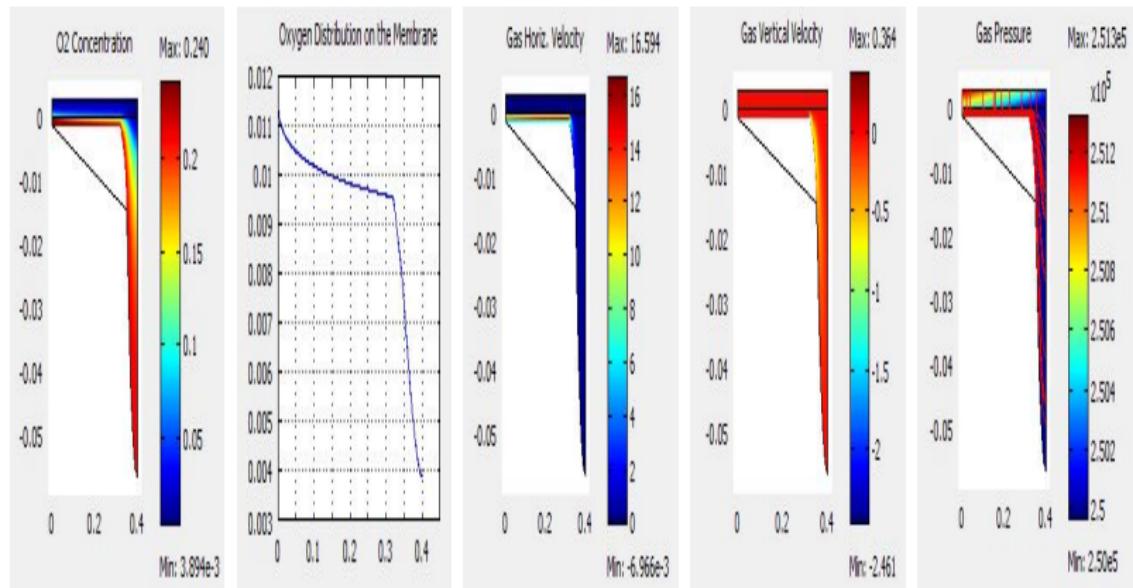
Numerical computations: w_v

- $w_u = w_1 = 0$, $w_v = 1$, $w_p = 0$



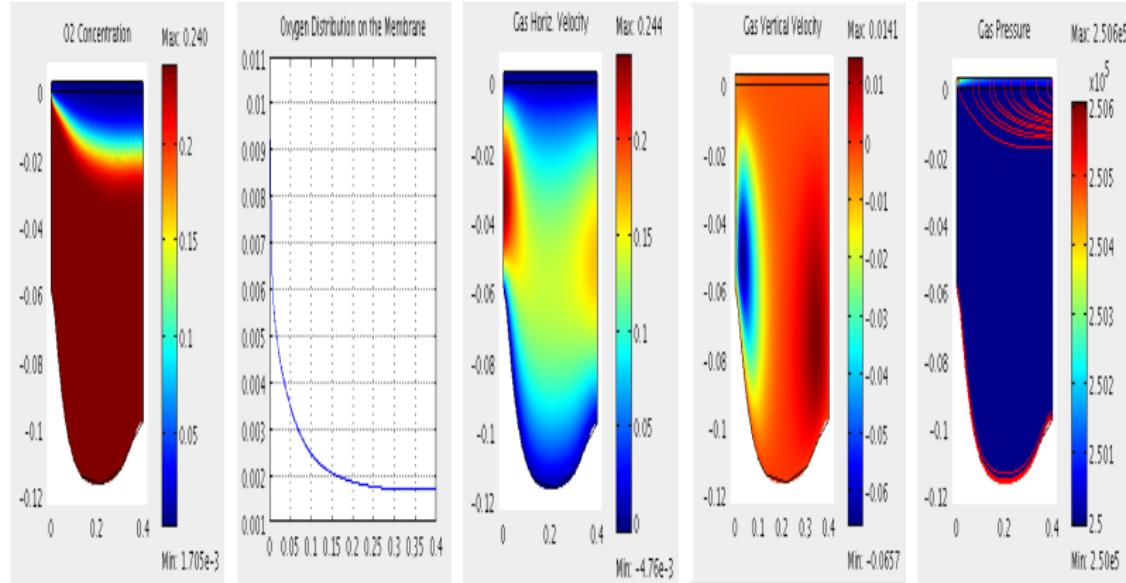
Numerical computations: w_v

- $w_u = w_1 = 0$, $w_v = 1$, $w_p = 0$



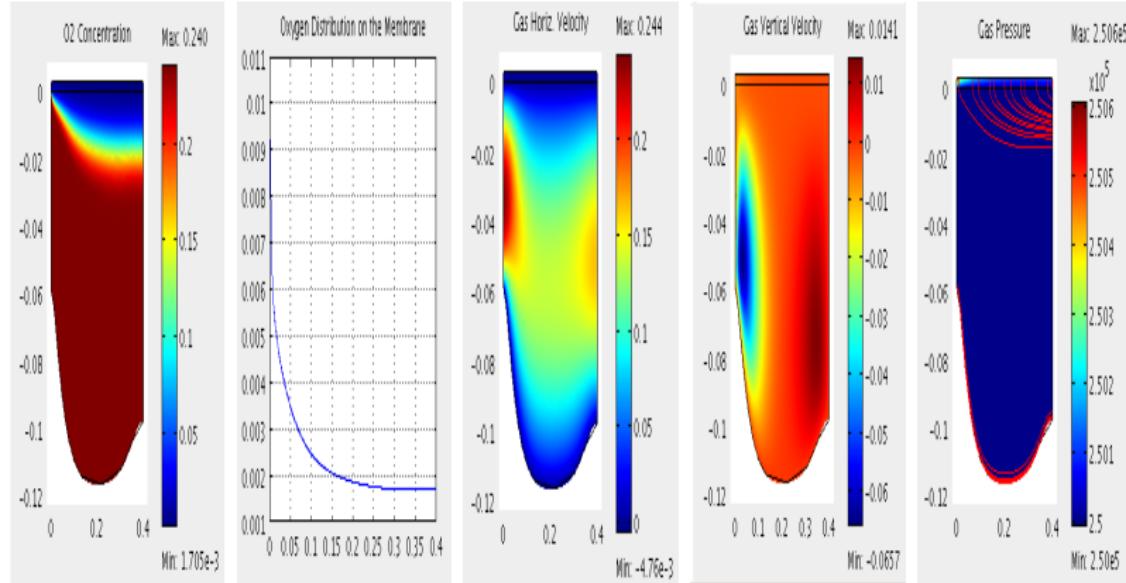
Numerical computations: w_p

- $w_u = w_1 = w_v = 0, w_p = 1$



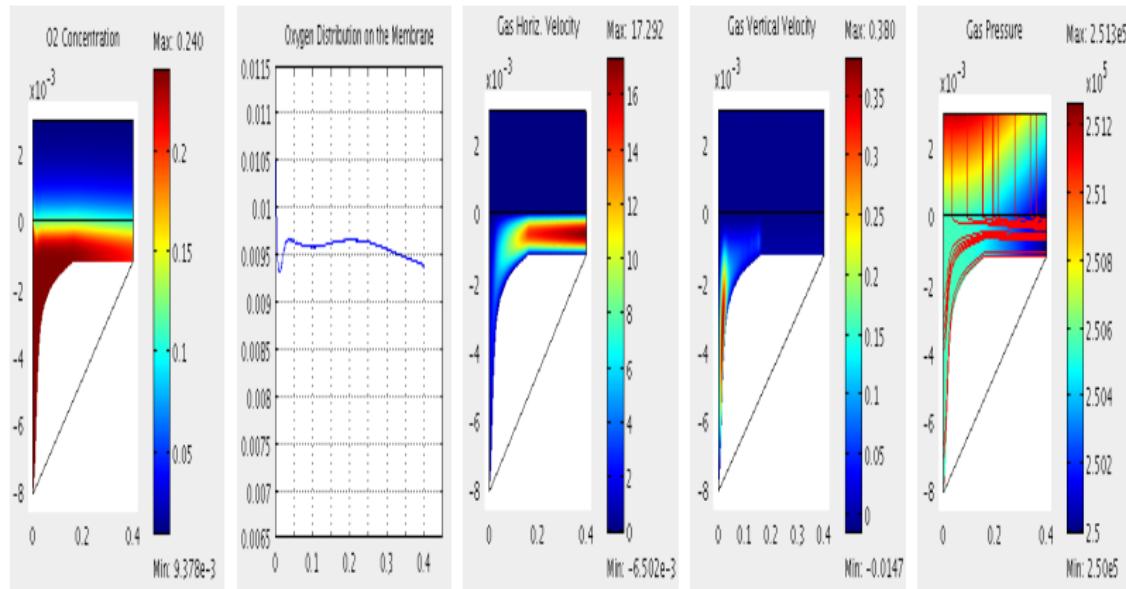
Numerical computations: w_p

- $w_u = w_1 = w_v = 0, w_p = 1$



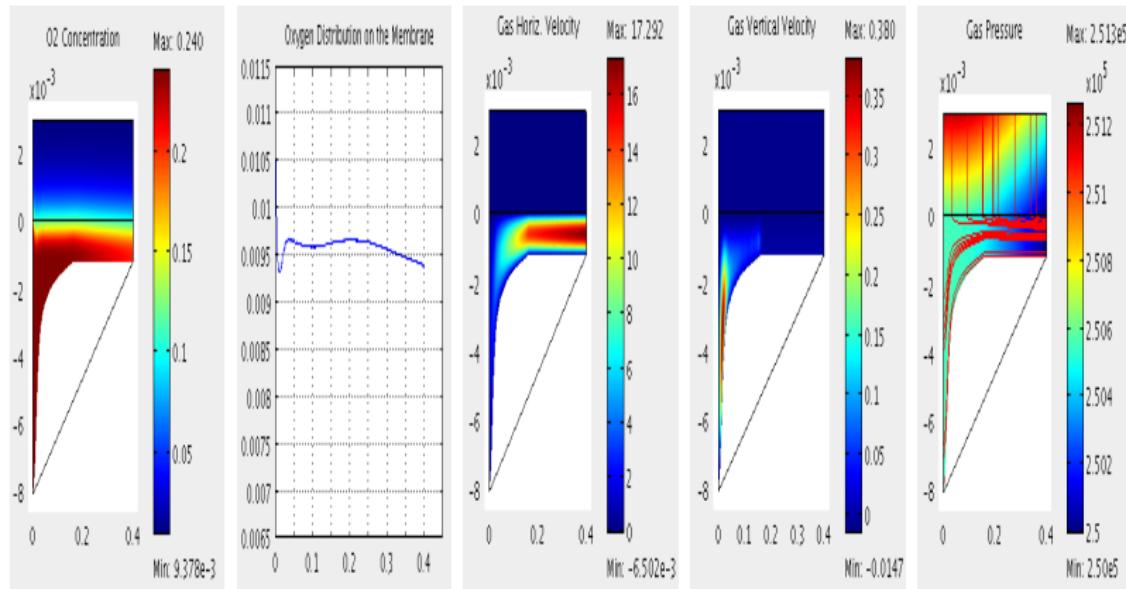
Numerical computations: w_u , w_1

- $w_u = 10^4$, $w_1 = 1$, $w_v = w_p = 0$



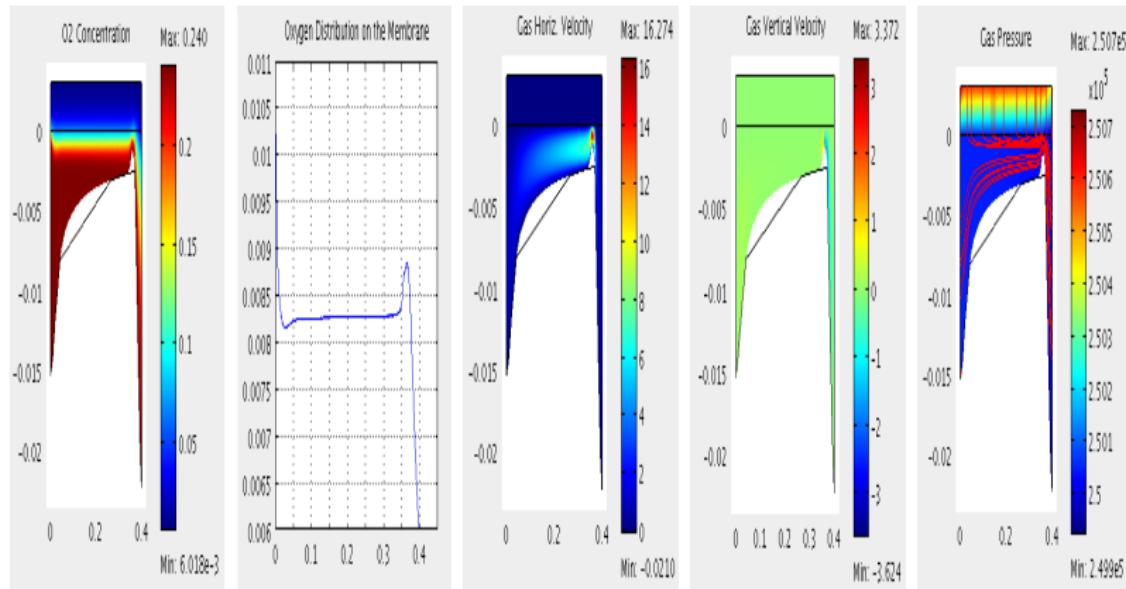
Numerical computations: w_u , w_1

- $w_u = 10^4$, $w_1 = 1$, $w_v = w_p = 0$



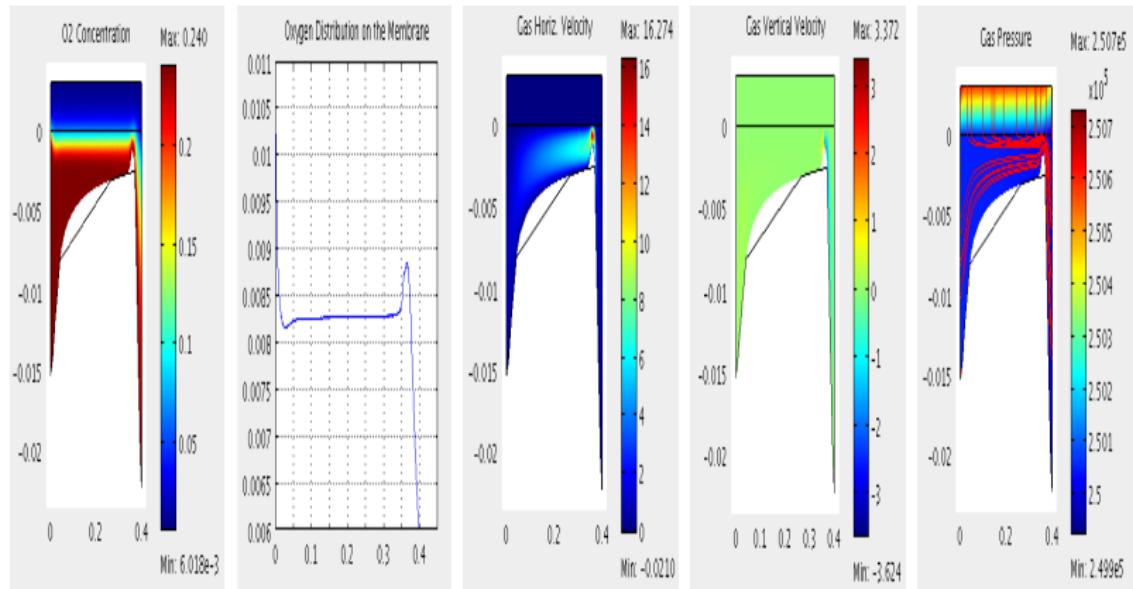
Numerical computations: w_u , w_v

- $w_u = 10^4$, $w_v = 1$, $w_1 = w_p = 0$



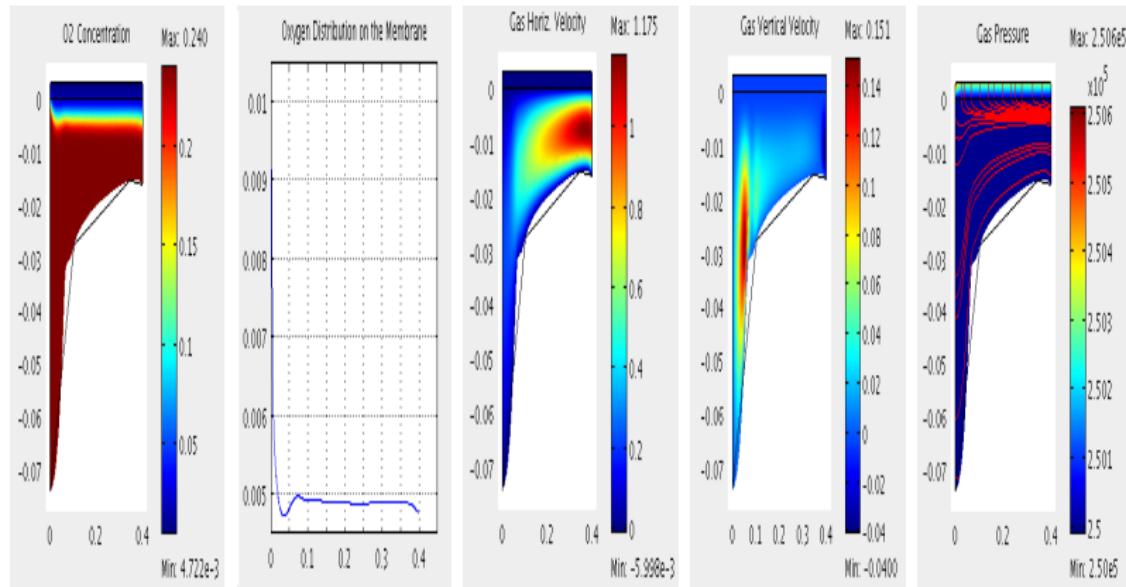
Numerical computations: w_u , w_v

- $w_u = 10^4$, $w_v = 1$, $w_1 = w_p = 0$



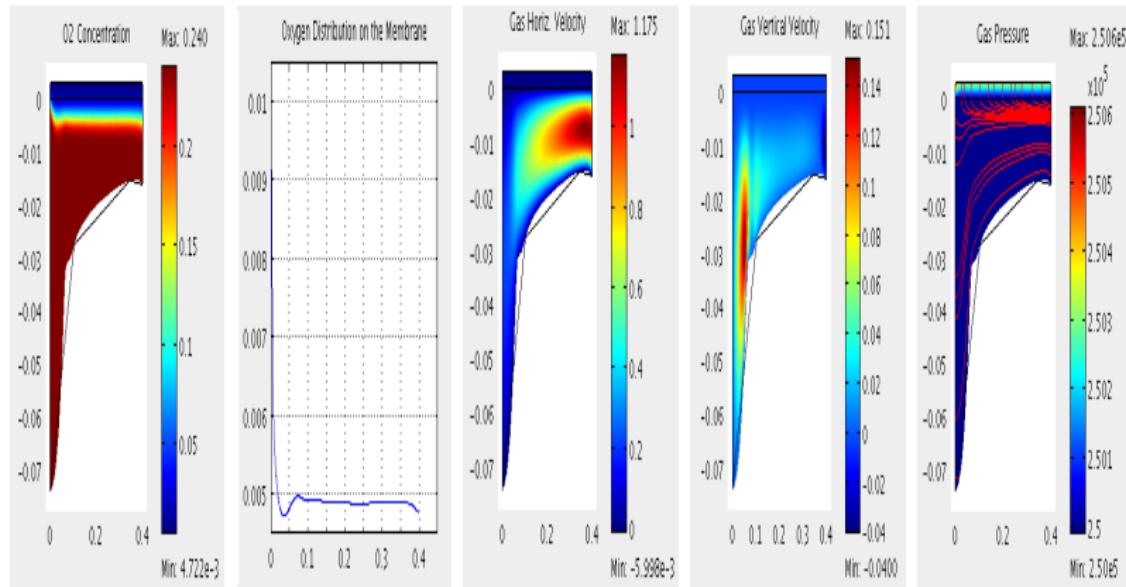
Numerical computations: w_u , w_p

- $w_u = 10^7$, $w_p = 1$, $w_1 = w_v = 0$



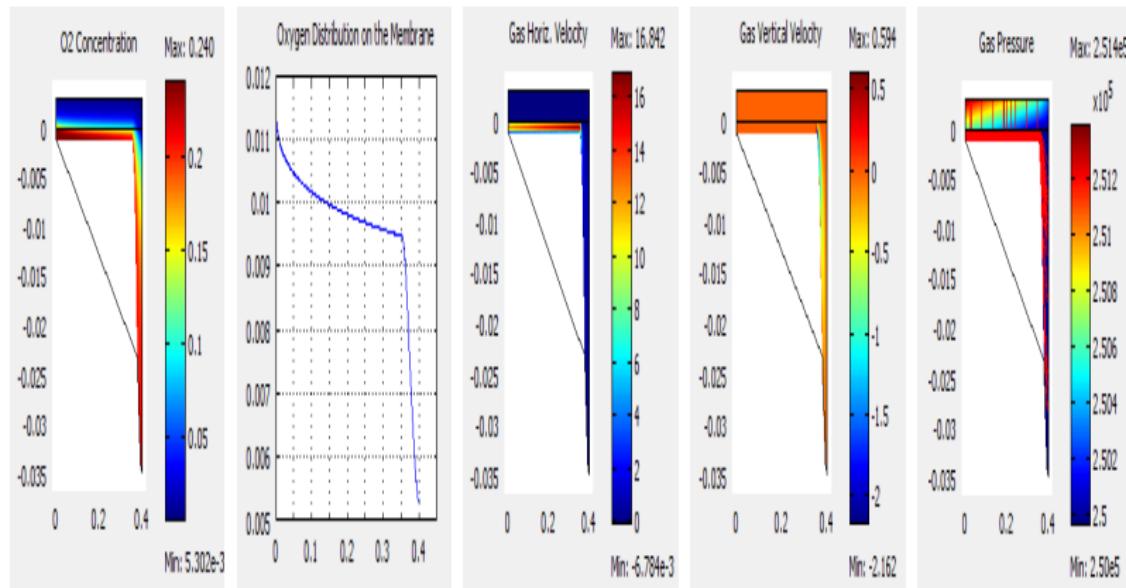
Numerical computations: w_u , w_p

- $w_u = 10^7$, $w_p = 1$, $w_1 = w_v = 0$



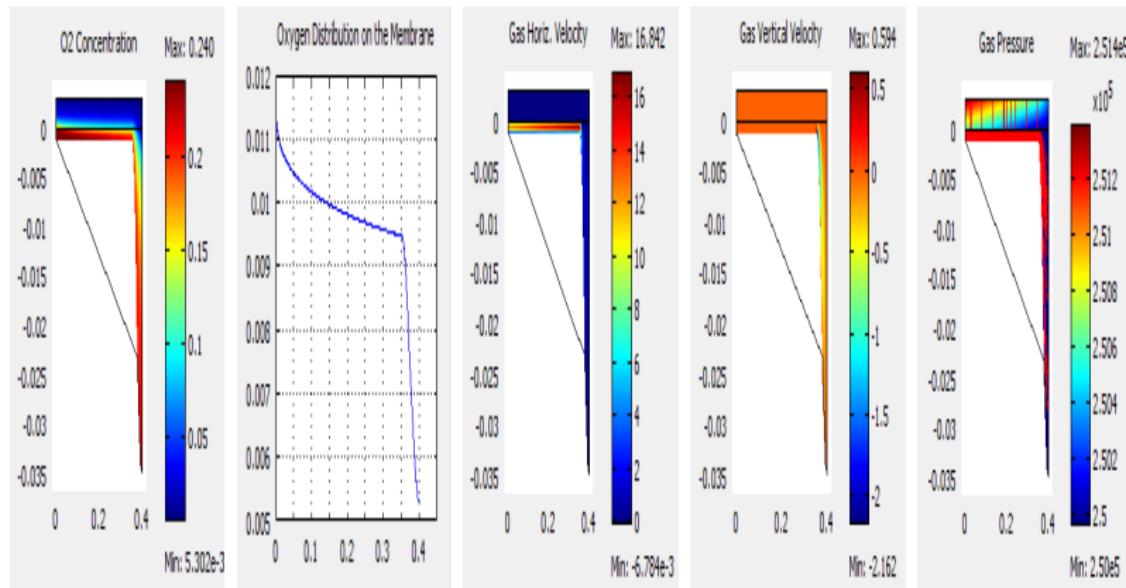
Numerical computations: w_1 , w_v

- $w_1 = 1$, $w_v = 1$, $w_u = w_p = 0$



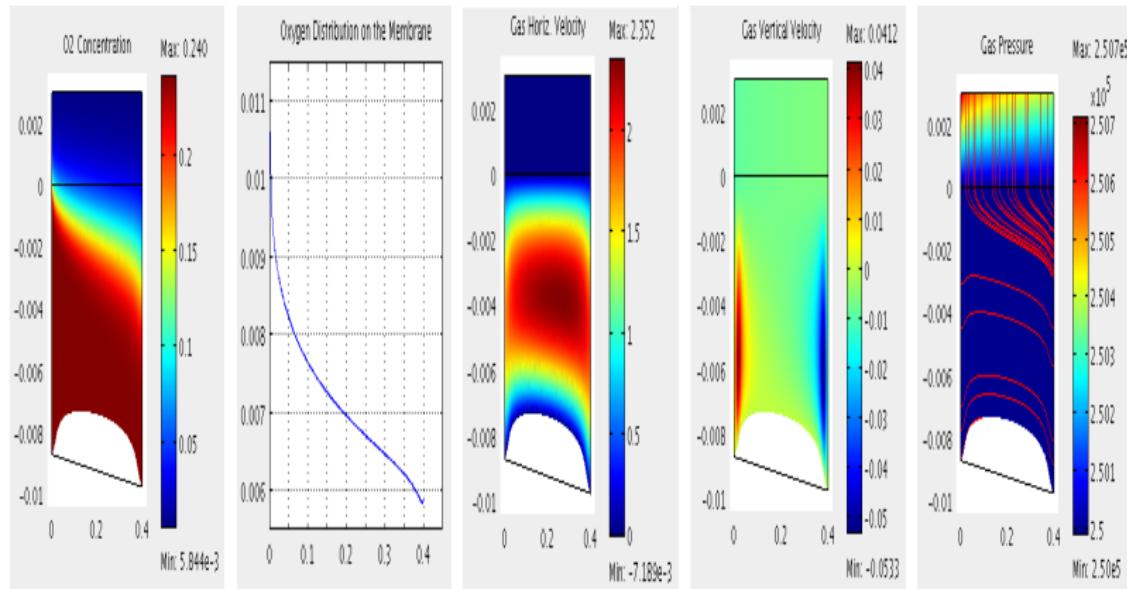
Numerical computations: w_1 , w_v

- $w_1 = 1$, $w_v = 1$, $w_u = w_p = 0$



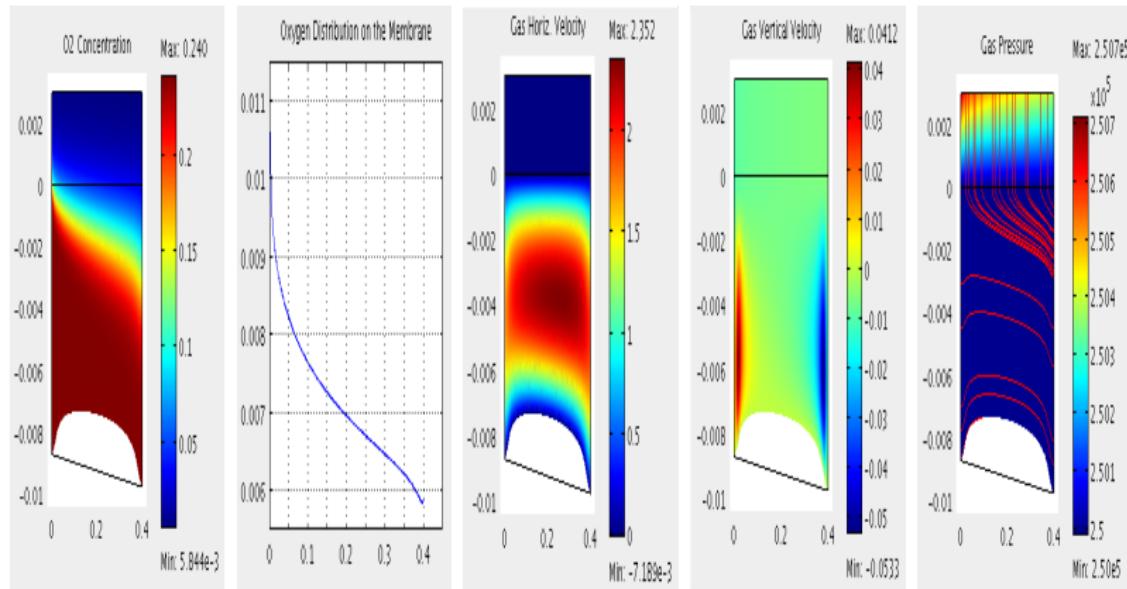
Numerical computations: w_1 , w_p

- $w_u = 10^7$, $w_p = 1$, $w_1 = w_v = 0$



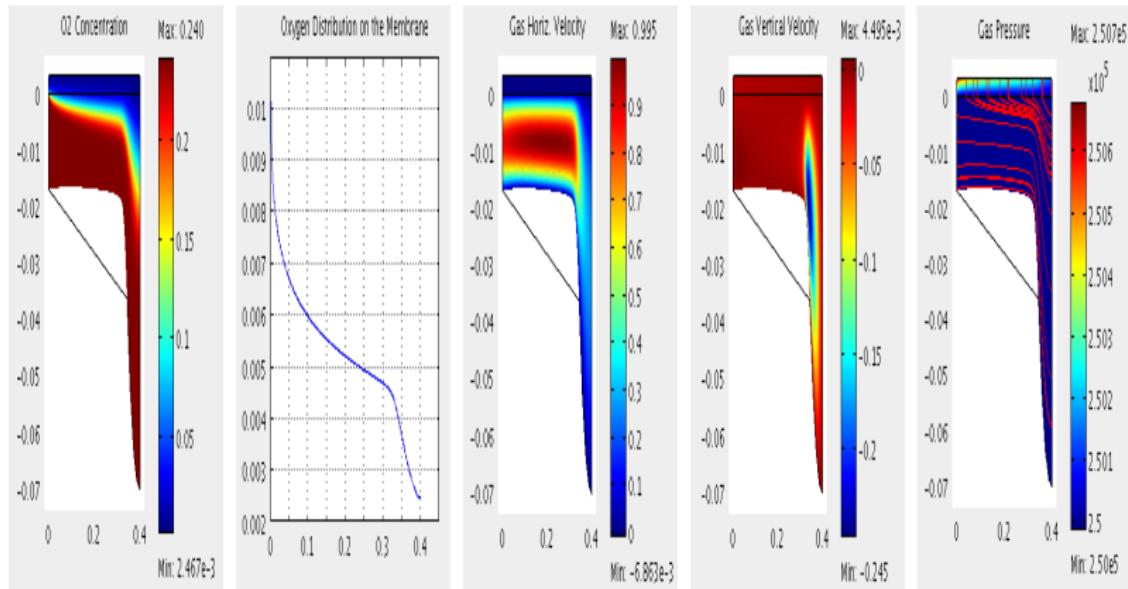
Numerical computations: w_1 , w_p

- $w_u = 10^7$, $w_p = 1$, $w_1 = w_v = 0$



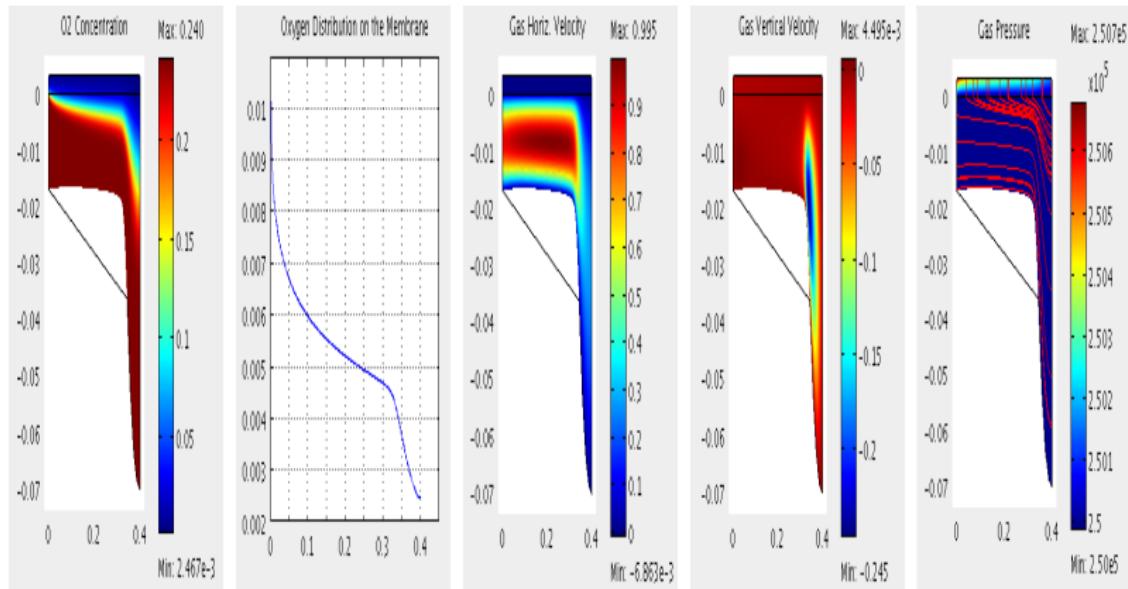
Numerical computations: w_v , w_p

- $w_v = 10^3$, $w_p = 1$, $w_1 = w_v = 0$



Numerical computations: w_v , w_p

- $w_v = 10^3$, $w_p = 1$, $w_1 = w_v = 0$



Thank you