

A Mathematical Model for Hydrogen Production of a Proton Exchange Membrane Photoelectrochemical Cell

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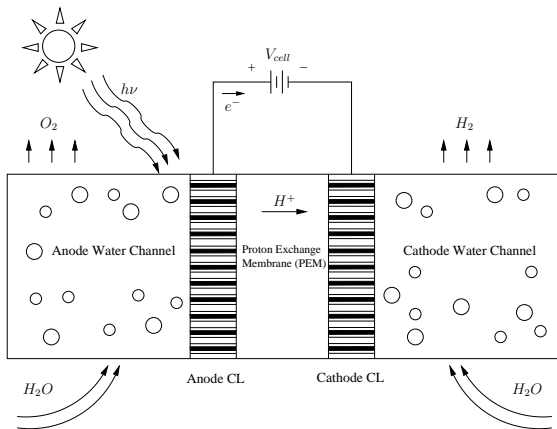
Benefits of Hydrogen

- Little or no emissions
- Hydrogen engines more efficient than gasoline
- Fuel cells available
- Many ways to produce

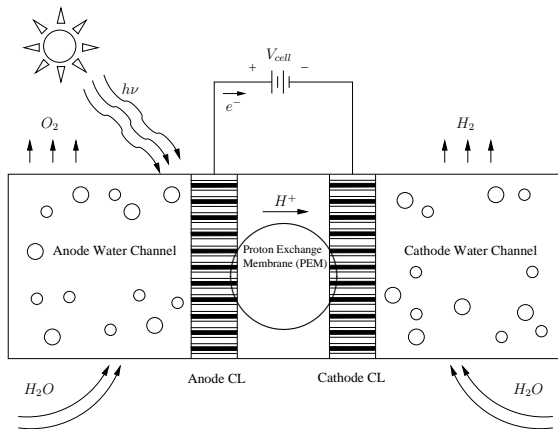
Ways to Produce Hydrogen

- Natural gas
- Coal
- Biomass
- Waste
- Wind
- Nuclear power
- Sunlight

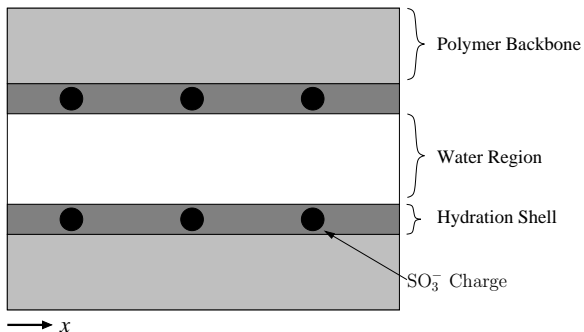
Basic Cell Operation



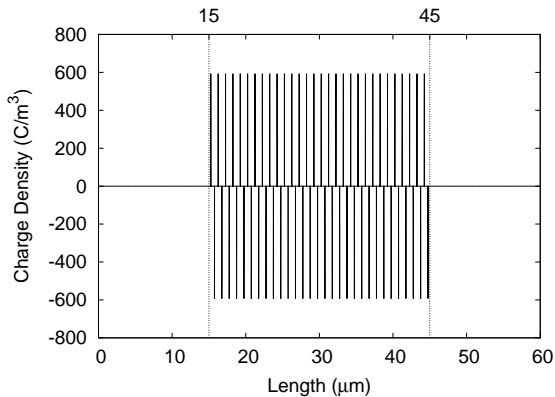
Basic Cell Operation



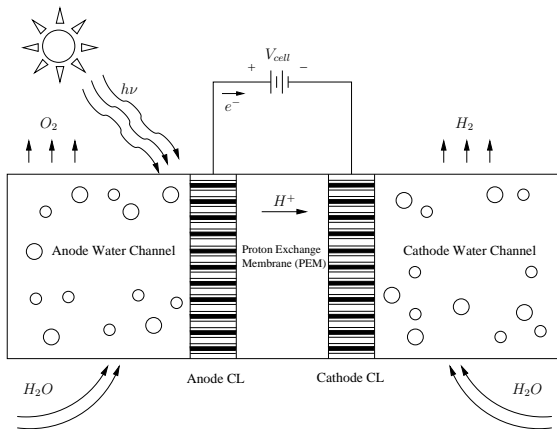
Nafion Membrane



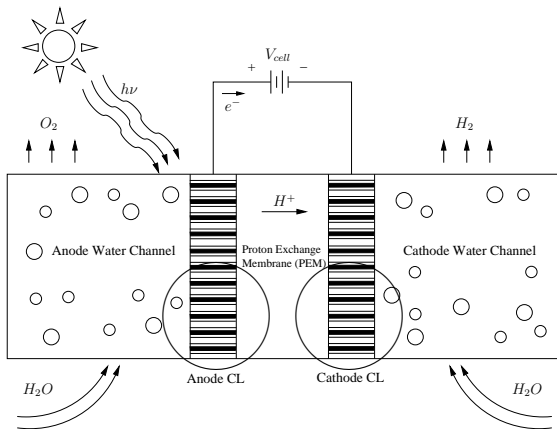
Delta Functions



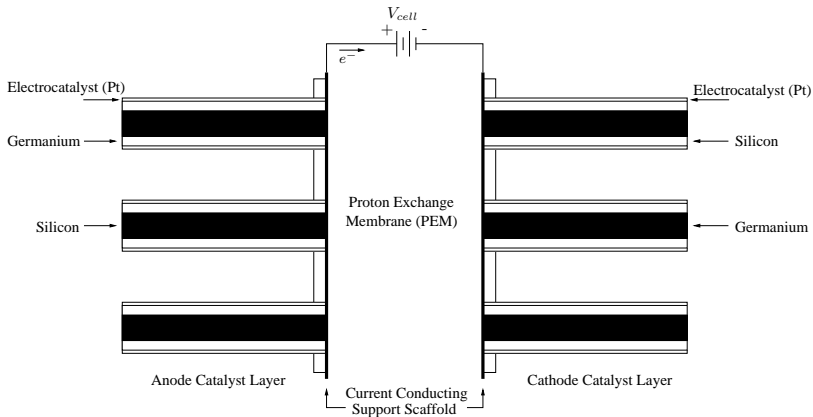
Basic Cell Operation



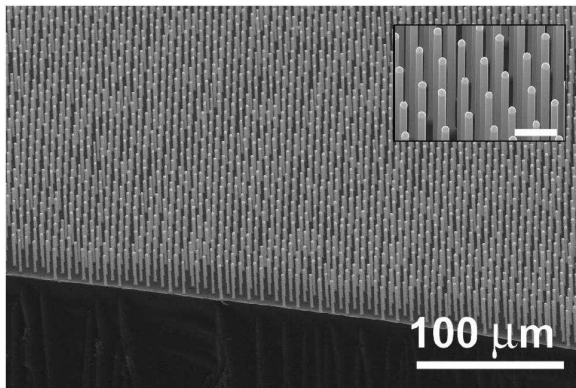
Basic Cell Operation



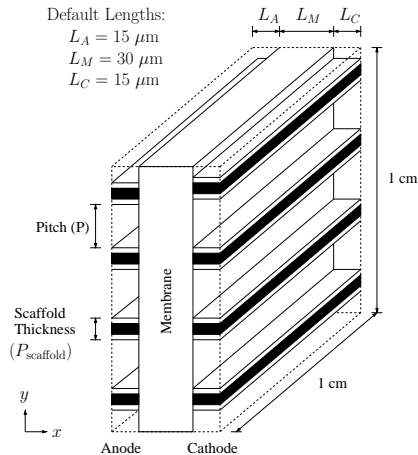
Electrode Nanowire Array Assembly



Photograph of Nanowire Arrays



Electrode Nanowire Array Assembly



Symbol	Description	Symbol	Description
A	Surface area/volume ratio [m^{-1}]	pos	Position of point-charges
c	Speed of light [m/s]	q	Charge of a proton [C]
D	Diffusivity of protons [m^2/s]	R	Gas constant [$\text{J/K}\cdot\text{mol}$]
D_w	Diffusivity of water [m^2/s]	S	Source/Sink term
E	Activation energy [J/mol]	T	Temperature [K]
EW	Equivalent weight of electrolyte [kg/mol]	W	Molecular weight [kg/mol]
F	Faraday constant [C/mol]	V	Volume [m^3]
h	Planck constant [$\text{m}^2\cdot\text{kg/s}$]	V_0	Equilibrium potential [V]
I_ν	Radiant intensity [W/m^2]	η	Overpotential [V]
j	Current density [A/m^2]	μ	Mobility of protons [$\text{m}^2/\text{V}\cdot\text{s}$]
J	Flux	ρ	Density [kg/m^3]
k_B	Boltzmann constant [J/K]	κ	Thermal conductivity [$\text{W/m}\cdot\text{K}$]
L	Length [m]	σ	Ionic conductivity [S/m]
m	Mass of an electron [kg]	ϵ	Permittivity [F/m]
N_A	Avogadro constant [mol^{-1}]	ν	Frequency of sunlight [Hz]
$N_{\text{SO}_3^-}$	Number of SO_3^- charges	χ	Surface potential difference [J]
n	Concentration of protons [mol/m^3]	ϕ_{metal}	Work function of metal [J]

	Governing Equation
Concentration of H ⁺	$0 = \nabla \cdot (D \nabla n + \mu n \nabla \Phi) + S$
Potential (CLs)	$0 = \nabla \cdot (\sigma \nabla \Phi) + S$
Potential (Membrane)	$0 = \nabla \cdot (\epsilon \nabla \Phi) + S$
Water Content	$0 = \nabla \cdot \left(\frac{\rho^{mem}}{EW} D_w^{mem} \nabla \lambda \right) - \nabla \cdot \left(n_d \frac{j}{F} \right) + S$
Temperature	$0 = \nabla \cdot (\kappa \nabla T) + S$

D - Diffusivity of protons

n - Concentration of protons

μ - Mobility of protons

σ - Electrical conductivity

Φ - Electric potential

ϵ - Permittivity

ρ^{mem} - Density of membrane

EW - Equiv. weight of dry membrane

D_w^{mem} - Diffusivity of water

λ - Water content

n_d - Electro-osmotic drag

j - Current density

F - Faraday constant

κ - Thermal conductivity

T - Temperature

	Governing Equation
Concentration of H ⁺	$0 = \frac{d}{dx} \left(D \frac{dn}{dx} + \mu n \frac{d\Phi}{dx} \right) + S$
Potential (CLs)	$0 = \frac{d}{dx} \left(\sigma \frac{d\Phi}{dx} \right) + S$
Potential (Membrane)	$0 = \frac{d}{dx} \left(\epsilon \frac{d\Phi}{dx} \right) + S$
Water Content	$0 = \frac{d}{dx} \left(\frac{\rho^{mem}}{EW} D_w^{mem} \frac{d\lambda}{dx} \right) - \frac{d}{dx} \left(n_d \frac{j}{F} \right) + S$
Temperature	$0 = \frac{d}{dx} \left(\kappa \frac{dT}{dx} \right) + S$

D - Diffusivity of protons

n - Concentration of protons

μ - Mobility of protons

σ - Electrical conductivity

Φ - Electric potential

ϵ - Permittivity

ρ^{mem} - Density of membrane

EW - Equiv. weight of dry membrane

D_w^{mem} - Diffusivity of water

λ - Water content

n_d - Electro-osmotic drag

j - Current density

F - Faraday constant

κ - Thermal conductivity

T - Temperature

Current Density

$$j_{\nu} = \frac{Fl_{\nu}}{N_A} \frac{mc^2}{h^2\nu^2} \left(1 - \frac{\phi_{metal} + \chi}{h\nu} \right) \quad (\text{Light})$$

$$j_{applied} = i_{A_0} \left[\exp\left(\frac{F\eta_A}{RT}\right) - \exp\left(-\frac{F\eta_A}{RT}\right) \right] \quad (\text{Anode})$$

$$j_{applied} = i_{C_0} \left[\frac{n}{n_{ref}} \exp\left(-\frac{F\eta_C}{RT}\right) - \frac{n}{n_{ref}} \exp\left(\frac{F\eta_C}{RT}\right) \right] \quad (\text{Cathode})$$

Overpotentials

$$\eta_A = \frac{RT}{F} \sinh^{-1} \left(\frac{j_{\text{applied}}}{2i_{A_0}} \right) \quad (\text{Anode})$$

$$\eta_C = -\frac{RT}{F} \sinh^{-1} \left(\frac{j_{\text{applied}} \frac{n_{\text{ref}}}{\bar{n}_C}}{2i_{C_0}} \right) \quad (\text{Cathode})$$

$$\eta_M = \frac{L_M j}{\sigma} \quad (\text{Membrane})$$

$$\eta_I = .05 V_0 \quad (\text{Interface})$$

$$V_0 = 1.23 - .9 \times 10^{-3} (T - 298.15) \quad (\text{Equilibrium Potential})$$

$$\phi_0 = V_0 + \eta_A - \eta_C + \eta_M + \eta_I \quad (\text{Cell Voltage})$$

Other Equations

$$\sigma = (.5139\lambda - .326) \exp \left[1268 \left(\frac{1}{303} - \frac{1}{T} \right) \right] \quad (\text{Conductivity})$$

$$D = 8 \times 10^{-10} \lambda - 3.1 \times 10^{-9} \quad (\text{Diffusivity})$$

$$\mu = \frac{Dq}{k_B T} \quad (\text{Mobility})$$

$$R_{H_2} = \frac{\bar{n}_C}{n_{ref}} \frac{j}{F} \quad \left[\frac{\text{mol}}{\text{m}^2 \text{ s}} \right]$$

$$= \frac{\bar{n}_C}{n_{ref}} \frac{j}{F} \frac{W_{H_2}}{\rho_{H_2}} \frac{V_C}{P + P_{scaffold}} \quad \left[\frac{\text{L}}{\text{s}} \right]$$

Electric Potential - Governing Equation

$$0 = (\sigma \Phi_x)_x + S$$

$$0 = \sigma \Phi_{xx} + \sigma_x \Phi_x + S$$

$$0 = \frac{\sigma}{\Delta x^2} [\Phi_{i-1} - 2\Phi_i + \Phi_{i+1}] + \frac{1}{4\Delta x^2} [\sigma_{i+1} - \sigma_{i-1}] [\Phi_{i+1} - \Phi_{i-1}] + S$$

Electric Potential - Matrix Equation

$$\begin{aligned}
 & [1] \Phi_{i-1} \\
 + & [-2] \Phi_i = -\frac{\Delta x^2}{\sigma_i} S - \frac{1}{4\sigma_i} (\sigma_{i+1} - \sigma_{i-1}) (\Phi_{i+1} - \Phi_{i-1}) \\
 & + [1] \Phi_{i+1}
 \end{aligned}$$

Electric Potential - Boundary Conditions

Left Boundary $x = x_A = 0$	Anode/Membrane $x = x_{AM}$	Membrane/Cathode $x = x_{MC}$	Right Boundary $x = x_C$
$\Phi_A = V_0 + \eta_A - \eta_C + \eta_M + \eta_I$	$\Phi_A = \Phi_M + \frac{\eta_I}{2}$ $\epsilon_A \nabla \Phi_A \cdot \hat{n} = \epsilon_M \nabla \Phi_M \cdot \hat{n}$	$\Phi_M = \Phi_C + \frac{\eta_I}{2}$ $\epsilon_M \nabla \Phi_M \cdot \hat{n} = \epsilon_C \nabla \Phi_C \cdot \hat{n}$	$\Phi_C = 0$

Electric Potential - Boundary Conditions

$$\epsilon_1 \frac{d\Phi_1}{dx} = \epsilon_2 \frac{d\Phi_2}{dx}$$

$$\frac{\epsilon_1}{2\Delta x} [\Phi_{i-2} - 4\Phi_{i-1} + 3\Phi_i] = \frac{\epsilon_2}{2\Delta x} [-3\Phi_i + 4\Phi_{i+1} - \Phi_{i+2}]$$

Electric Potential - Boundary Conditions

$$\begin{aligned} & [\epsilon_1] \Phi_{i-2} \\ & + [-4\epsilon_1] \Phi_{i-1} \\ + & [3(\epsilon_1 + \epsilon_2)] \Phi_i = 0 \\ & + [-4\epsilon_2] \Phi_{i+1} \\ & + [\epsilon_1] \Phi_{i+2} \end{aligned}$$

Concentration of Hydrogen - Governing Equation

$$\begin{aligned}
 n_t &= (Dn_x + \mu n \Phi_x)_x + S \\
 \frac{1}{\Delta t} [n_i^{k+1} - n_i^k] &= \frac{D_i}{2\Delta x^2} [(n_{i-1}^k - 2n_i^k + n_{i+1}^k) + (n_{i-1}^{k+1} - 2n_i^{k+1} + n_{i+1}^{k+1})] \\
 &+ \frac{1}{8\Delta x^2} [D_{i+1} - D_{i-1}] [(n_{i+1}^k - n_{i-1}^k) + (n_{i+1}^{k+1} - n_{i-1}^{k+1})] \\
 &+ \frac{\mu_i}{2\Delta x^2} [n_i^{k+1} - n_i^k] [\Phi_{i-1} - 2\Phi_i + \Phi_{i+1}] \\
 &+ \frac{\mu_i}{8\Delta x^2} [(n_{i+1}^k - n_{i-1}^k) + (n_{i+1}^{k+1} - n_{i-1}^{k+1})] [\Phi_{i+1} - \Phi_{i-1}] \\
 &+ \frac{1}{8\Delta x^2} [\mu_{i+1} - \mu_{i-1}] [n_i^{k+1} - n_i^k] [\Phi_{i+1} - \Phi_{i-1}] \\
 &+ S_i^k
 \end{aligned}$$

Concentration of Hydrogen - Matrix Equation

$$\begin{aligned}
 & \left[-\frac{\tilde{r}}{2}D_i + \frac{\tilde{r}}{8}(D_{i+1} + D_{i-1}) + \frac{\tilde{r}}{8}\mu_i(\Phi_{i+1} - \Phi_{i-1}) \right] n_{i-1}^{k+1} \\
 + & \left[1 + \tilde{r}D_i - \frac{\tilde{r}}{2}\mu_i(\Phi_{i+1} - 2\Phi_i + \Phi_{i-1}) - \frac{\tilde{r}}{8}(\mu_{i+1} - \mu_{i-1})(\Phi_{i+1} - \Phi_{i-1}) \right] n_i^{k+1} \\
 + & \left[-\frac{\tilde{r}}{2}D_i - \frac{\tilde{r}}{8}(D_{i+1} - D_{i-1}) - \frac{\tilde{r}}{8}\mu_i(\Phi_{i+1} - \Phi_{i-1}) \right] n_{i+1}^{k+1} \\
 = & n_i^k + \frac{\tilde{r}}{2}D_i(n_{i-1}^k - 2n_i^k + n_{i+1}^k) + \frac{\tilde{r}}{8}(D_{i+1} - D_{i-1})(n_{i+1}^k - n_{i-1}^k) \\
 & + \frac{\tilde{r}}{2}\mu_i n_i^k (\Phi_{i-1} - 2\Phi_i + \Phi_{i+1}) + \frac{\tilde{r}}{8}\mu_i(\Phi_{i+1} - \Phi_{i-1})(n_{i+1}^k - n_{i-1}^k) \\
 & - \frac{\tilde{r}}{8}n_i^k(\mu_{i+1} - \mu_{i-1})(\Phi_{i+1} - \Phi_{i-1}) + \Delta t S_i^k
 \end{aligned}$$

Concentration of Hydrogen - Boundary Conditions

Left Boundary $x = x_A = 0$	Anode/Membrane $x = x_{AM}$	Membrane/Cathode $x = x_{MC}$	Right Boundary $x = x_C$
$n_A = n_0$	$n_A = n_M$ $\vec{J}_A \cdot \hat{n} = \vec{J}_M \cdot \hat{n}$	$n_M = n_C$ $\vec{J}_M \cdot \hat{n} = \vec{J}_C \cdot \hat{n}$	$\vec{J}_C \cdot \hat{n} = K_{MT}[n_C - n_0]$

$$\vec{J} = D \nabla n - \mu n \nabla \Phi$$

Concentration of Hydrogen - Boundary Conditions

$$D_1 \frac{dn_1}{dx} + \mu_1 n_1 \frac{d\Phi_1}{dx} = D_2 \frac{dn_2}{dx} + \mu_2 n_2 \frac{d\Phi_2}{dx}$$

$$\begin{aligned} \frac{D_1}{2\Delta x} [n_{i-2} - 4n_{i-1} + 3n_i] + \frac{\mu_1 n_i}{2\Delta x} [\Phi_{i-2} - 4\Phi_{i-1} + 3\Phi_i] \\ = \frac{D_2}{2\Delta x} [-3n_i + 4n_{i+1} - n_{i+2}] + \frac{\mu_2 n_i}{2\Delta x} [-3\Phi_i + 4\Phi_{i+1} - \Phi_{i+2}] \end{aligned}$$

Concentration of Hydrogen - Boundary Conditions

$$\begin{aligned}
 & [D_1] n_{i-2} \\
 & + [-4D_1] n_{i-1} \\
 & + [3(D_1 + D_2) + \mu_1(\Phi_{i-2} - 4\Phi_{i-1} + 3\Phi_i) \\
 & \quad - \mu_2(-3\Phi_i + 4\Phi_{i+1} - \Phi_{i+2})] n_i = 0 \\
 & + [-4D_2] n_{i+1} \\
 & + [D_2] n_{i+2}
 \end{aligned}$$

$$\begin{aligned}
 & [D_i] n_{i-2} \\
 & + [-4D_i] n_{i-1} \\
 & + [3D_i + \mu_i(\Phi_{i-2} - 4\Phi_{i-1} + 3\Phi_i) - 2K_{MT}\Delta x] n_i = -2K_{MT}n_0\Delta x \\
 & + [-4D_2] n_{i+1} \\
 & + [D_2] n_{i+2}
 \end{aligned}$$

Temperature - Governing Equation

$$0 = (\kappa T_x)_x + S$$

$$0 = \kappa T_{xx} + S$$

$$0 = \frac{\kappa}{\Delta x^2} [T_{i-1} - 2T_i + T_{i+1}] + S$$

Temperature - Matrix Equation

$$\begin{aligned} & [\kappa] T_{i-1} \\ + & [-2\kappa] T_i = -\Delta x^2 S \\ & + [\kappa] T_{i+1} \end{aligned}$$

Temperature - Boundary Conditions

Left Boundary	Anode/Membrane	Membrane/Cathode	Right Boundary
$x = x_A = 0$	$x = x_{AM}$	$x = x_{MC}$	$x = x_C$
$T_A = T_0$	$T_A = T_M$ $\nabla T_A \cdot \hat{n} = \nabla T_M \cdot \hat{n}$	$T_M = T_C$ $\nabla T_M \cdot \hat{n} = \nabla T_C \cdot \hat{n}$	$T_C = T_0$

Temperature - Boundary Conditions

$$\kappa_1 \frac{dT_1}{dx} = \kappa_2 \frac{dT_2}{dx}$$

$$\frac{\kappa_1}{2\Delta x^2} [T_{i-2} - 4T_{i-1} + 3T_i] = \frac{\kappa_2}{2\Delta x^2} [-3T_i + 4T_{i+1} - T_{i+2}]$$

Temperature - Boundary Conditions

$$\begin{aligned} & [\kappa_1] T_{i-2} \\ & + [-4\kappa_1] T_{i-1} \\ & + [3(\kappa_1 + \kappa_2)] T_i = 0 \\ & + [-4\kappa_2] T_{i+1} \\ & + [\kappa_2] T_{i+2} \end{aligned}$$

Water Content - Governing Equation

$$0 = \left(\frac{\rho^{mem}}{EW} D_w \lambda_x \right)_x - \left(n_d \frac{j}{F} \right)_x + S, \quad n_d = \frac{2.5}{22} \lambda$$

$$\begin{aligned} 0 = & \frac{\rho^{mem}}{EW} \frac{D_{w_i}}{\Delta x^2} [\lambda_{i-1} - 2\lambda_i + \lambda_{i+1}] \\ & + \frac{\rho^{mem}}{EW} \frac{1}{4\Delta x^2} [D_{w_{i+1}} - D_{w_{i-1}}] [\lambda_{i+1} - \lambda_{i-1}] \\ & - \frac{2.5}{22} \frac{i}{F} \frac{1}{2\Delta x} [\lambda_{i+1} - \lambda_{i-1}] \end{aligned}$$

Water Content - Matrix Equation

$$\begin{aligned}
 & \left[\frac{\rho^{mem}}{EW} \left(D_{w_i} - \frac{D_{w_{i+1}} - D_{w_{i-1}}}{4} \right) + \Delta x \frac{2.5}{22} \frac{i}{F} \right] \lambda_{i-1} \\
 & \quad + \left[-2 \frac{\rho^{mem}}{EW} D_{w_i} \right] \lambda_i = -\Delta x^2 S \\
 & + \left[\frac{\rho^{mem}}{EW} \left(D_{w_i} + \frac{D_{w_{i+1}} - D_{w_{i-1}}}{4} \right) - \Delta x \frac{2.5}{22} \frac{i}{F} \right] \lambda_{i+1}
 \end{aligned}$$

Water Content - Boundary Conditions

Left Boundary $x = x_A = 0$	Anode/Membrane $x = x_{AM}$	Membrane/Cathode $x = x_{MC}$	Right Boundary $x = x_C$
$\lambda_A = \lambda_0$	$\lambda_A = \lambda_M$ $D_{wA} \nabla \lambda_A \cdot \hat{n}$ $= D_{wM} \nabla \lambda_M \cdot \hat{n}$	$\lambda_M = \lambda_C$ $D_{wM} \nabla \lambda_M \cdot \hat{n}$ $= D_{wC} \nabla \lambda_C \cdot \hat{n}$	$\lambda_C = \lambda_0$

Water Content - Boundary Conditions

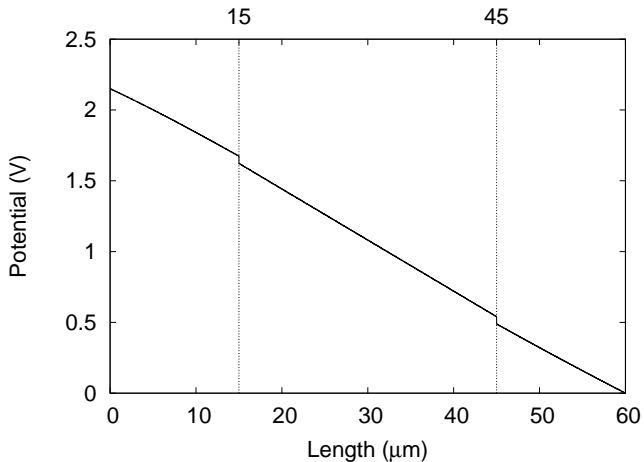
$$D_{w_1} \frac{d\lambda_1}{dx} = D_{w_2} \frac{d\lambda_2}{dx}$$

$$\frac{D_{w_1}}{4 \Delta x} [\lambda_{i-2} - 4\lambda_{i-1} + 3\lambda_i] = \frac{D_{w_2}}{4 \Delta x} [-3\lambda_i + 4\lambda_i - \lambda_{i+2}]$$

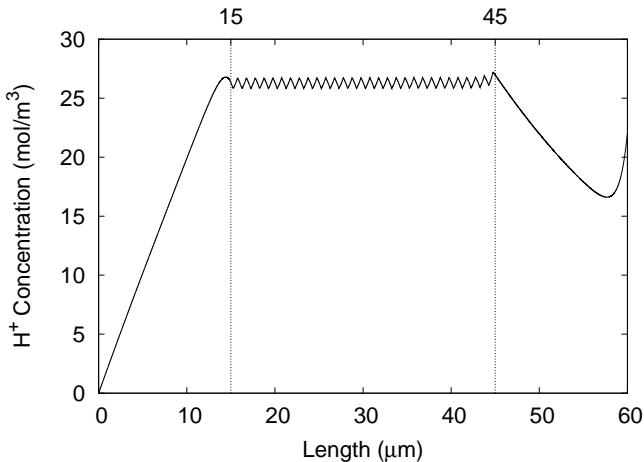
Water Content - Boundary Conditions

$$\begin{aligned} & [D_{w_1}] \lambda_{i-2} \\ & + [-4D_{w_1}] \lambda_{i-1} \\ + & [3(D_{w_1} + D_{w_2})] \lambda_i = 0 \\ & + [-4D_{w_2}] \lambda_{i+1} \\ & + [D_{w_2}] \lambda_{i+2} \end{aligned}$$

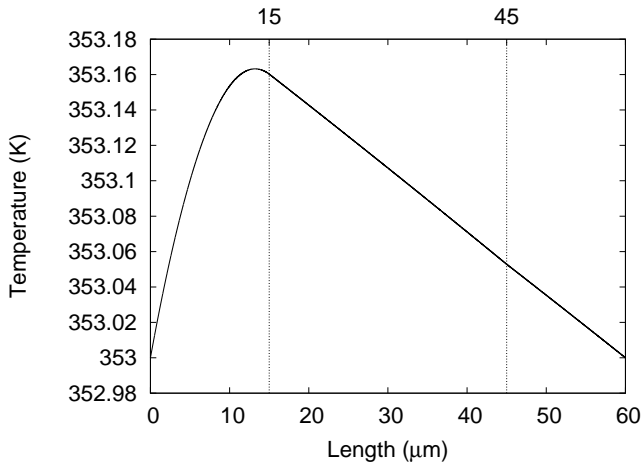
Default Electric Potential



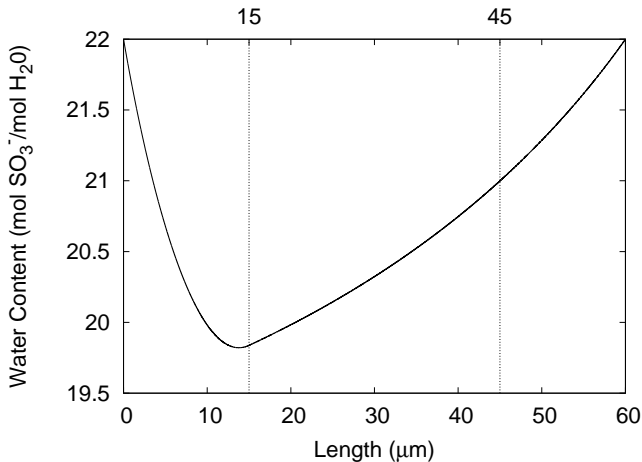
Default Hydrogen Concentration



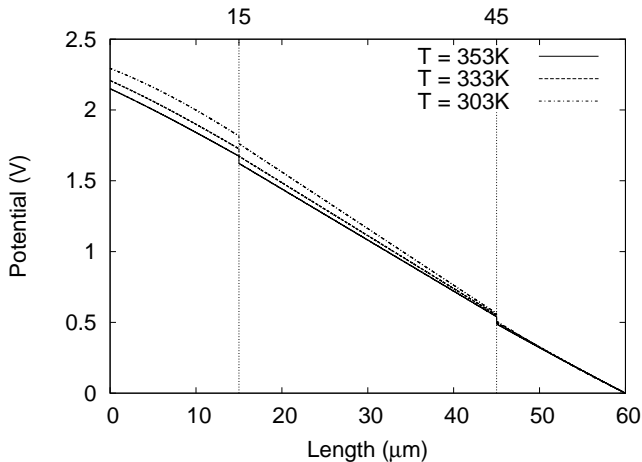
Default Temperature



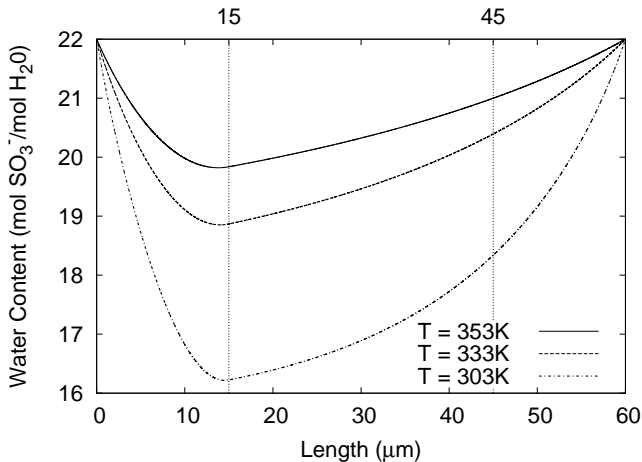
Default Water Content



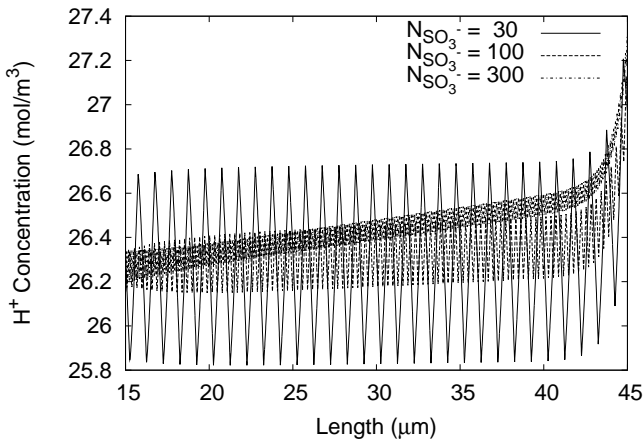
Effects of Temperature



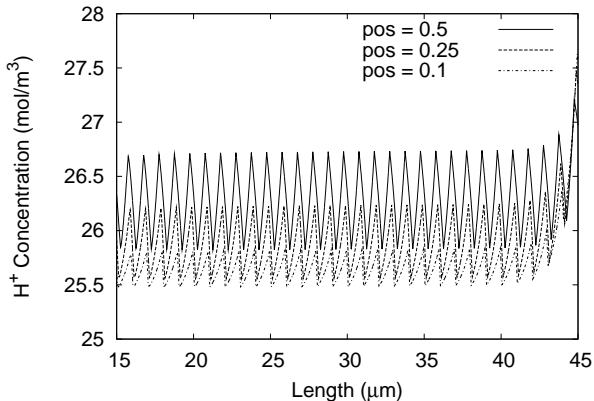
Effects of Temperature



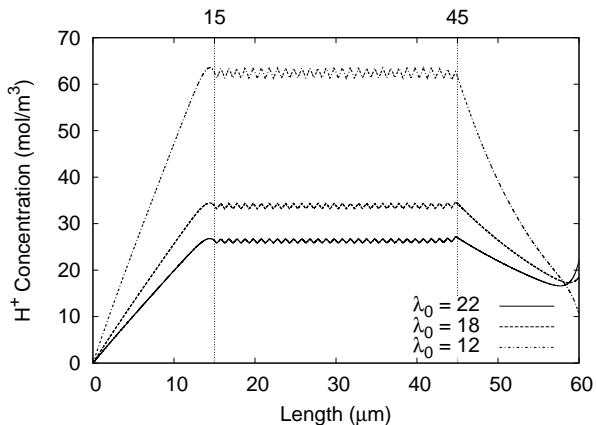
Effects of Charges in Membrane



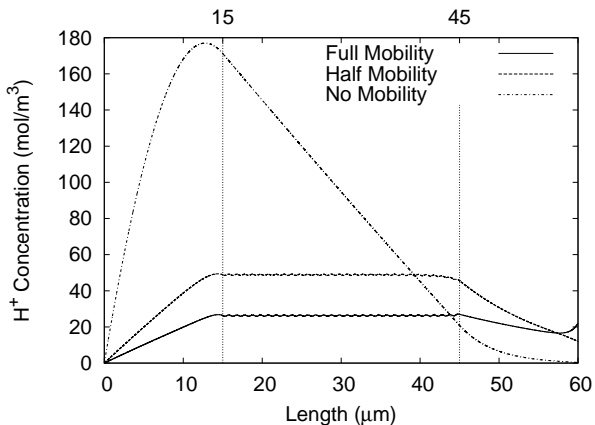
Effects of Charges in Membrane



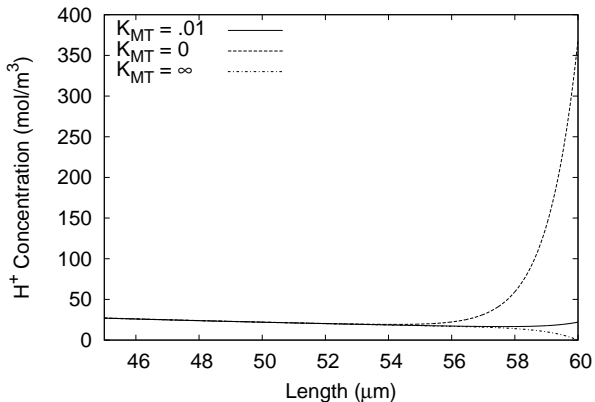
Effects of Water Content



Effects of Mobility



Effect of Mass Transfer Coefficient



Hydrogen Production (Part I)

Test Case	H ₂ Production	
	[ml/min]	% of Default
Default	5.9531	100.0 %
Low Temperature (T = 333K)	5.8859	98.9 %
Low Temperature (T = 303K)	6.0412	101.5 %
$\lambda_0 = 18$	6.8881	115.7 %
$\lambda_0 = 12$	9.4656	159.0 %
100 SO ₃ ⁻ and H ⁺ Charges	5.9714	100.3 %
300 SO ₃ ⁻ and H ⁺ Charges	6.0240	101.2 %
pos = .25	6.0044	100.9 %
pos = .1	6.0345	101.4 %
$K_{MT} = 0$	12.1445	204.0 %
$K_{MT} = \infty$	5.5605	93.4 %

Hydrogen Production (Part I)

Test Case	H ₂ Production	
	[ml/min]	% of Default
Default	5.9531	100.0 %
Low Temperature (T = 333K)	5.8859	98.9 %
Low Temperature (T = 303K)	6.0412	101.5 %
$\lambda_0 = 18$	6.8881	115.7 %
$\lambda_0 = 12$	9.4656	159.0 %
100 SO ₃ ⁻ and H ⁺ Charges	5.9714	100.3 %
300 SO ₃ ⁻ and H ⁺ Charges	6.0240	101.2 %
pos = .25	6.0044	100.9 %
pos = .1	6.0345	101.4 %
$K_{MT} = 0$	12.1445	204.0 %
$K_{MT} = \infty$	5.5605	93.4 %

Hydrogen Production (Part II)

Test Case	H ₂ Production	
	[ml/min]	% of Default
Default	5.9531	100.0 %
Half Mobility	7.5597	127.0 %
No Mobility	1.6420	27.6 %
$I_{\nu} = 0.6 \text{ mW/cm}^2$	5.9869	100.6 %
$I_{\nu} = 1.2 \text{ mW/cm}^2$	6.0556	101.7 %
$P = 5\mu\text{m}$	9.6349	161.8 %
$P = 3\mu\text{m}$	17.9736	301.9 %
$L_A = L_C = 10\mu\text{m}$	2.4909	41.8 %
$L_A = L_C = 30\mu\text{m}$	22.5301	378.5 %
$L_M = 20\mu\text{m}$	5.3653	90.1 %
$L_M = 40\mu\text{m}$	6.4290	108.0 %

Hydrogen Production (Part II)

Test Case	H ₂ Production	
	[ml/min]	% of Default
Default	5.9531	100.0 %
Half Mobility	7.5597	127.0 %
No Mobility	1.6420	27.6 %
$I_{\nu} = 0.6 \text{ mW/cm}^2$	5.9869	100.6 %
$I_{\nu} = 1.2 \text{ mW/cm}^2$	6.0556	101.7 %
$P = 5\mu\text{m}$	9.6349	161.8 %
$P = 3\mu\text{m}$	17.9736	301.9 %
$L_A = L_C = 10\mu\text{m}$	2.4909	41.8 %
$L_A = L_C = 30\mu\text{m}$	22.5301	378.5 %
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Significant Factors

- Electrode surface area
- Mass transfer coefficient between cathode and water channel
- Input water concentration

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Future Work

- Inclusion of water channels
- Multi-dimensional
- Non-linear channel flow
- Optimal mobility and diffusivity
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