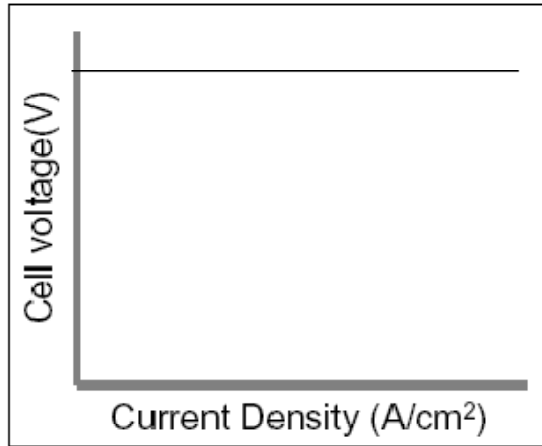
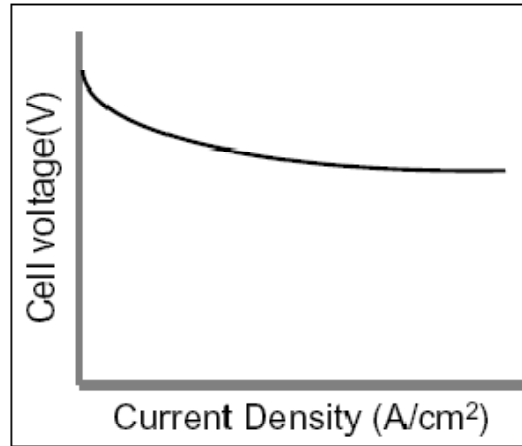


Losses in Fuel Cells

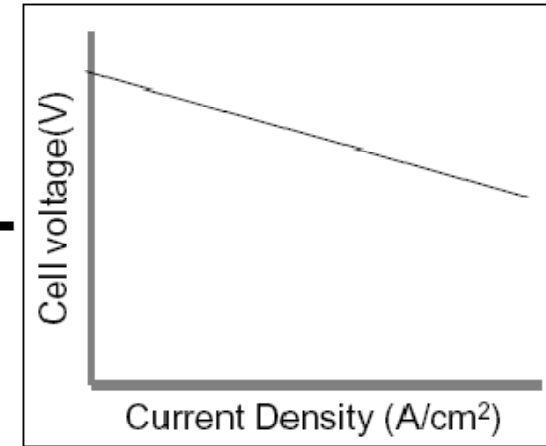
Reversible Voltage (Chapter 2)



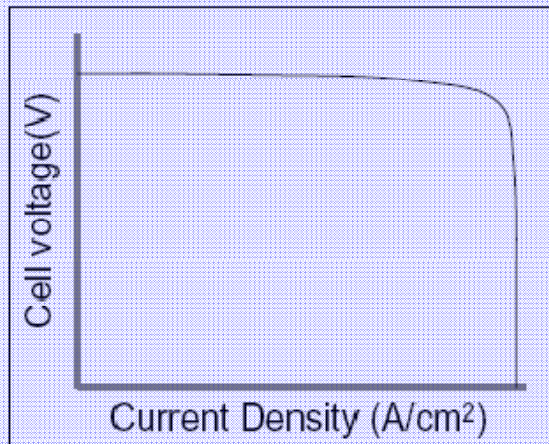
Rxn. Loss (Chapter 3)



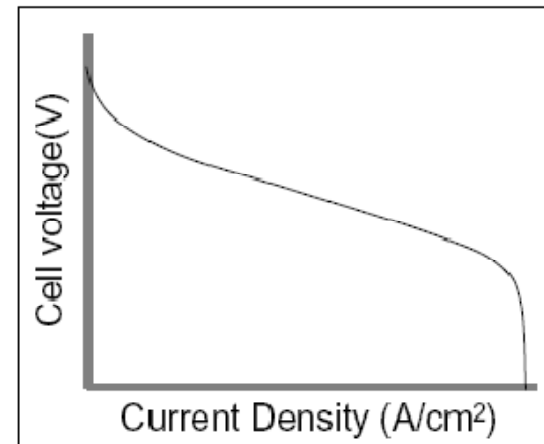
Ohmic Loss (Chapter 4)



Concentration Loss (Chapter 5)



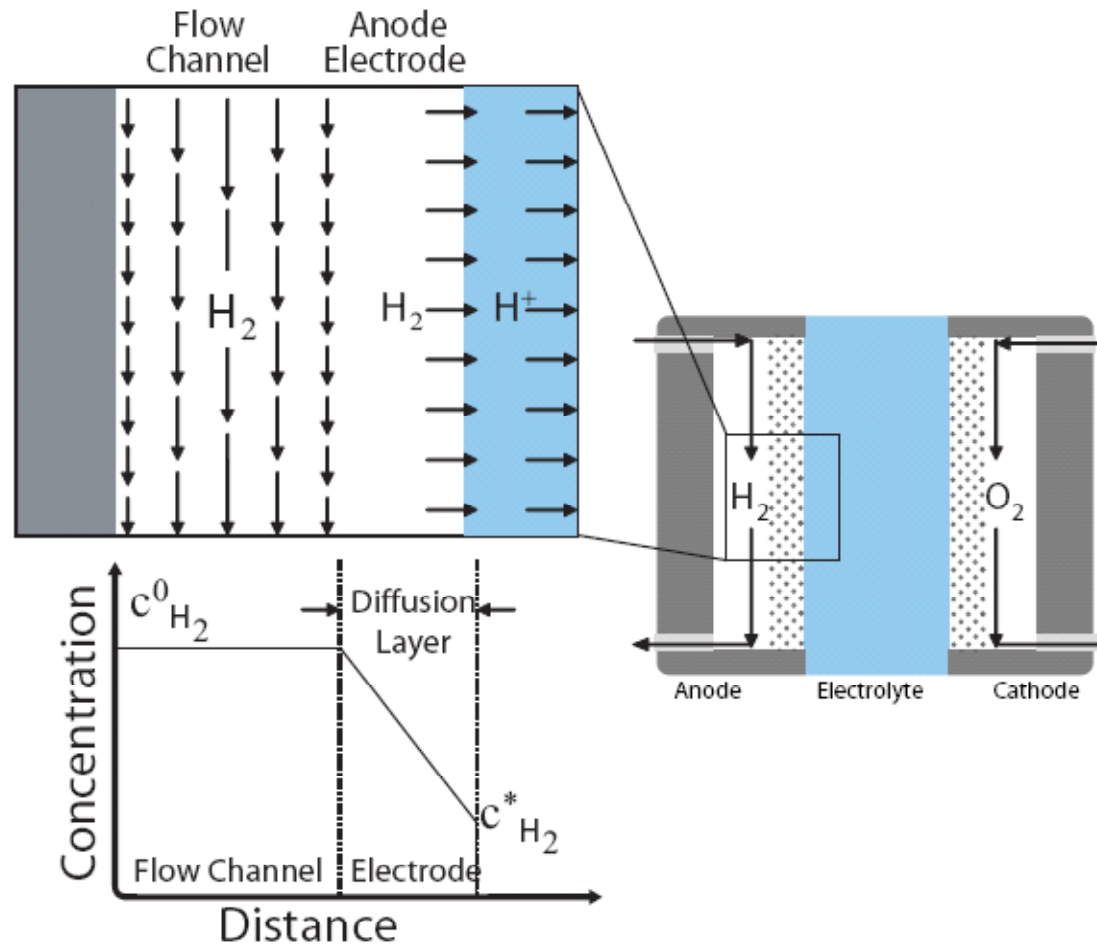
Net Fuel Cell Performance



$$V = E_{thermo} - \eta_{act} - \eta_{ohmic} - \eta_{conc}$$

Fuel Cell Charge Transport

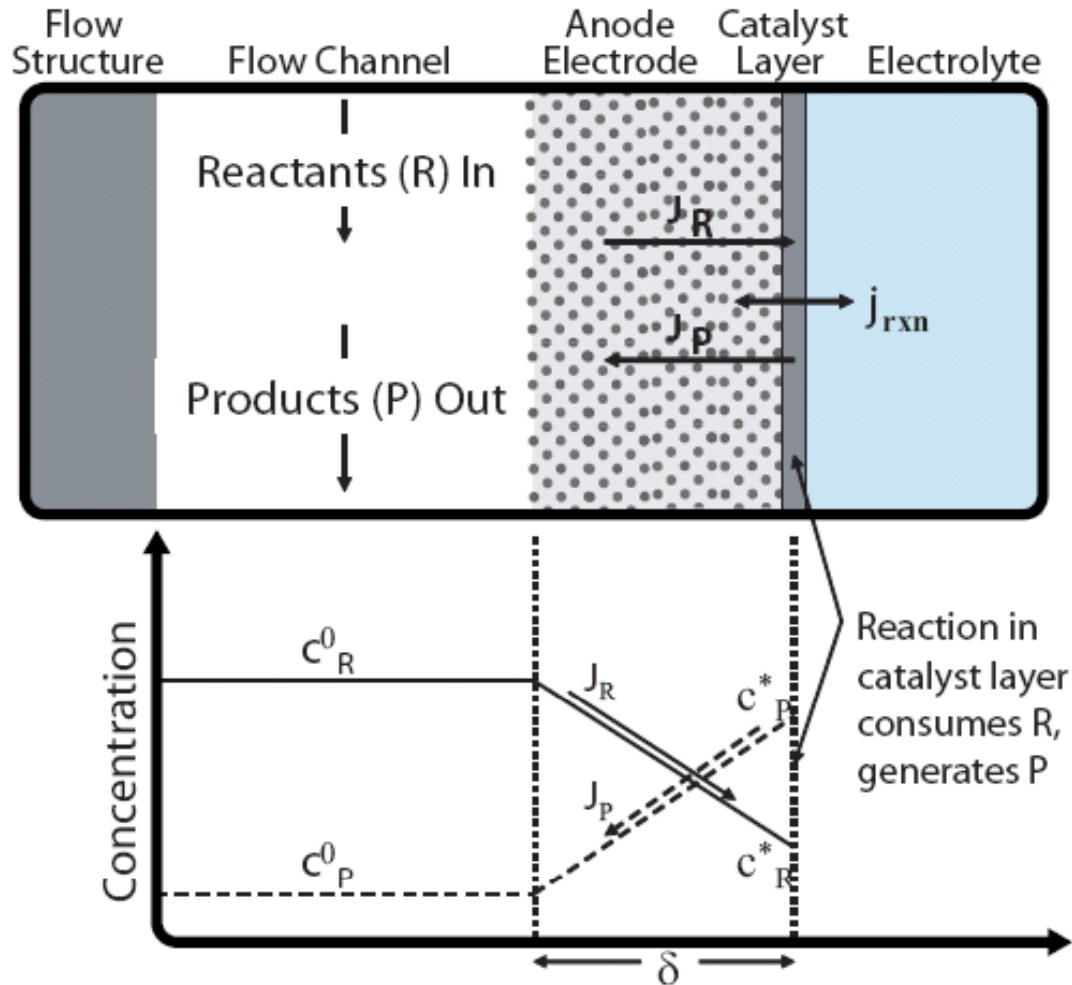
Mass Transport



Convection dominant in flow channels

Diffusion dominant in electrode

Concentration Drop



$$E = E^0 - \frac{RT}{nF} \ln \frac{\prod p_{\text{Product}}^{v_i}}{\prod p_{\text{Reactants}}^{v_i}}$$

$$j = j_0 \left(\frac{C_R}{C_R^0} e^{\left(\frac{\alpha n F \eta}{RT}\right)} - \frac{C_P}{C_P^0} e^{-\left(\frac{(1-\alpha) n F \eta}{RT}\right)} \right)$$

Diffusion In Electrode

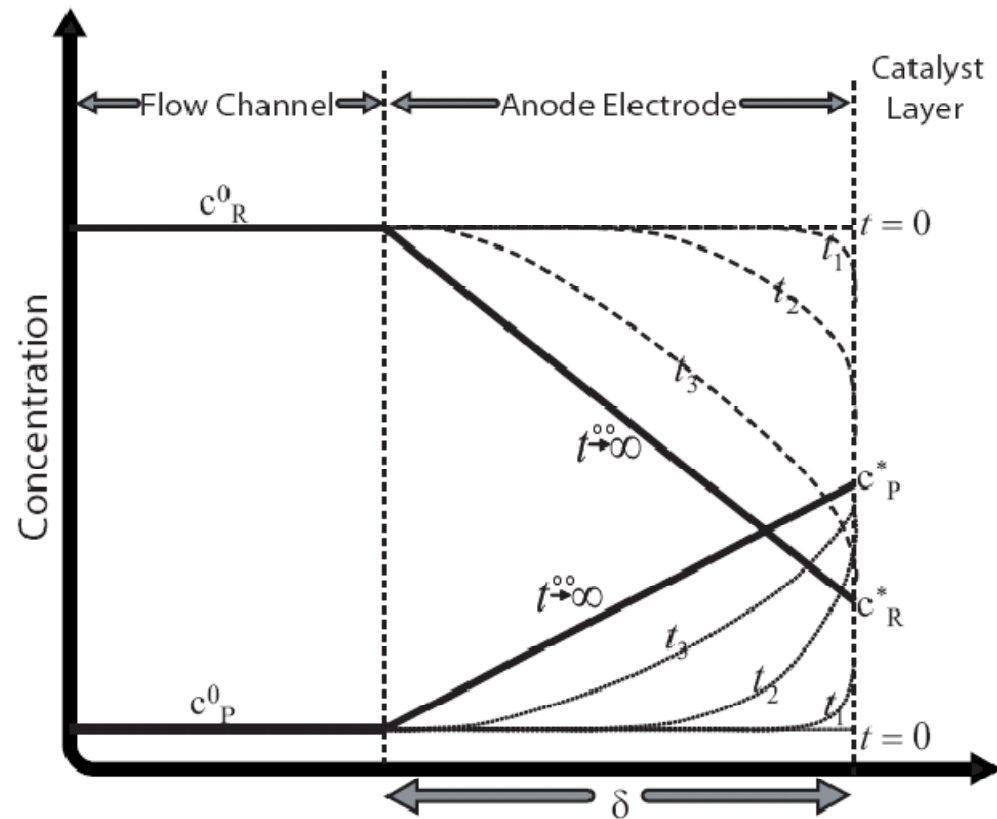
$$J_{diff} = -D \frac{dc}{dx}$$

$$J_{diff} = -D^{eff} \frac{c_R^* - c_R^0}{\delta}$$

$$j = nF J_{diff}$$

$$j = -nFD^{eff} \frac{c_R^* - c_R^0}{\delta}$$

$$c_R^* = c_R^0 - \frac{j\delta}{nFD^{eff}}$$



Limiting Current Density

$$j_L = nFD^{eff} \frac{c_R^0}{\delta}$$

Typical values for δ are around $100\text{--}300\mu\text{m}$ and D^{eff} are around $10^{-2}\text{cm}^2/\text{s}$. Therefore typical limiting current densities are on order of $1\text{--}10\text{A}/\text{cm}^2$. This

– To increase j_L

1. Ensuring a high c_R^0 (by designing good flow structures that evenly distribute reactants).
2. Ensuring that D^{eff} is large and δ is small (by carefully optimizing fuel cell operating conditions, electrode structure, and diffusion layer thickness).

Q: Are 1 & 2 are easy?

Q: Does anode has larger j_L ?

Diffusivity & Effective Diffusivity

Diffusivity from kinetic theory

$$p \cdot D_{ij} = a \left(\frac{T}{\sqrt{T_{ci}T_{cj}}} \right)^b (p_{ci}p_{cj})^{1/3} (T_{ci}T_{cj})^{5/12} \left(\frac{1}{M_i} + \frac{1}{M_j} \right)^{1/2}$$

Substance	Molecular Weight, M	$T_c(K)$	$p_c(\text{atm})$
H ₂	2.016	33.3	12.80
Air	28.964	132.4	37.0
N ₂	28.013	126.2	33.5
O ₂	31.999	154.4	49.7
CO	28.010	132.9	34.5
CO ₂	44.010	304.2	72.8
H ₂ O	18.015	647.3	217.5

Effective diffusivity

$$D_{ij}^{eff} = \epsilon^{1.5} D_{ij}$$

$$D_{ij}^{eff} = \epsilon^\tau D_{ij}$$

$$D_{ij}^{eff} = D_{ij} \frac{\epsilon}{\tau}$$

Nernst Effect

$$E = E^0 - \frac{RT}{nF} \ln \frac{\prod a_{PRODUCTS}^{v_i}}{\prod a_{REACTANTS}^{v_i}}$$

$$\eta_{conc} = E_{Nernst}^0 - E_{Nernst}^*$$

$$\eta_{conc} = \left(E^0 - \frac{RT}{nF} \ln \frac{1}{c_R^0} \right) - \left(E^0 - \frac{RT}{nF} \ln \frac{1}{c_R^*} \right)$$

$$\eta_{conc} = \frac{RT}{nF} \ln \frac{c_R^0}{c_R^*}$$

$$c_R^* = c_R^0 - \frac{j\delta}{nFD^{eff}}$$

$$c_R^* = \frac{j_L\delta}{nFD^{eff}} - \frac{j\delta}{nFD^{eff}}$$

$$\frac{c_R^0}{c_R^*} = \frac{\frac{j_L\delta}{nFD^{eff}}}{\frac{j_L\delta}{nFD^{eff}} - \frac{j\delta}{nFD^{eff}}}$$

$$\frac{c_R^0}{c_R^*} = \frac{j_L}{j_L - j}$$

$$\eta_{conc} = \frac{RT}{nF} \ln \frac{j_L}{j_L - j}$$

Concentration Effect

B-V for high current density

$$j = j_0^0 \left(\frac{c_R^*}{c_R^{0*}} e^{\left(\frac{\alpha n F \eta_{act}}{RT} \right)} \right)$$

$$\eta_{act} = \frac{RT}{\alpha n F} \ln \frac{j c_R^{0*}}{j_0^0 c_R^*}$$

$$\eta_{conc} = \eta_{act}^* - \eta_{act}^0$$

$$\eta_{conc} = \left(\frac{RT}{\alpha n F} \ln \frac{j c_R^{0*}}{j_0^0 c_R^*} \right) - \left(\frac{RT}{\alpha n F} \ln \frac{j c_R^{0*}}{j_0^0 c_R^0} \right)$$

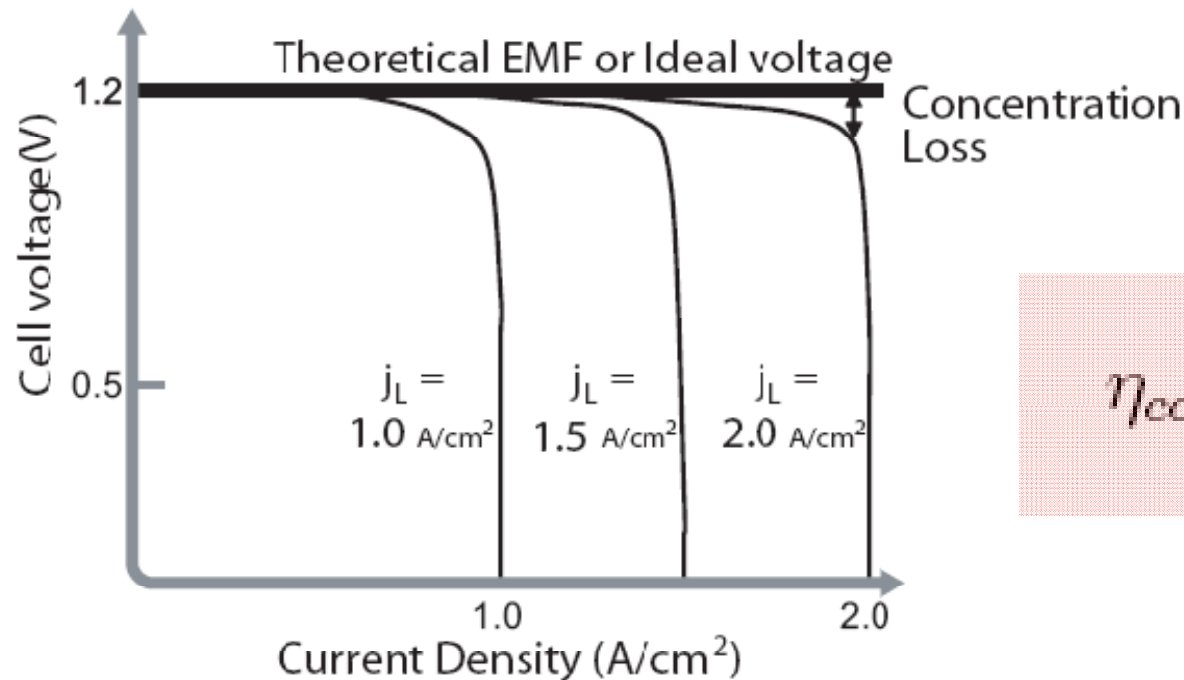
$$\eta_{conc} = \frac{RT}{\alpha n F} \ln \frac{c_R^0}{c_R^*}$$

$$\eta_{conc} = \frac{RT}{\alpha n F} \ln \frac{j_L}{j_L - j}$$

Mass Transportation Loss

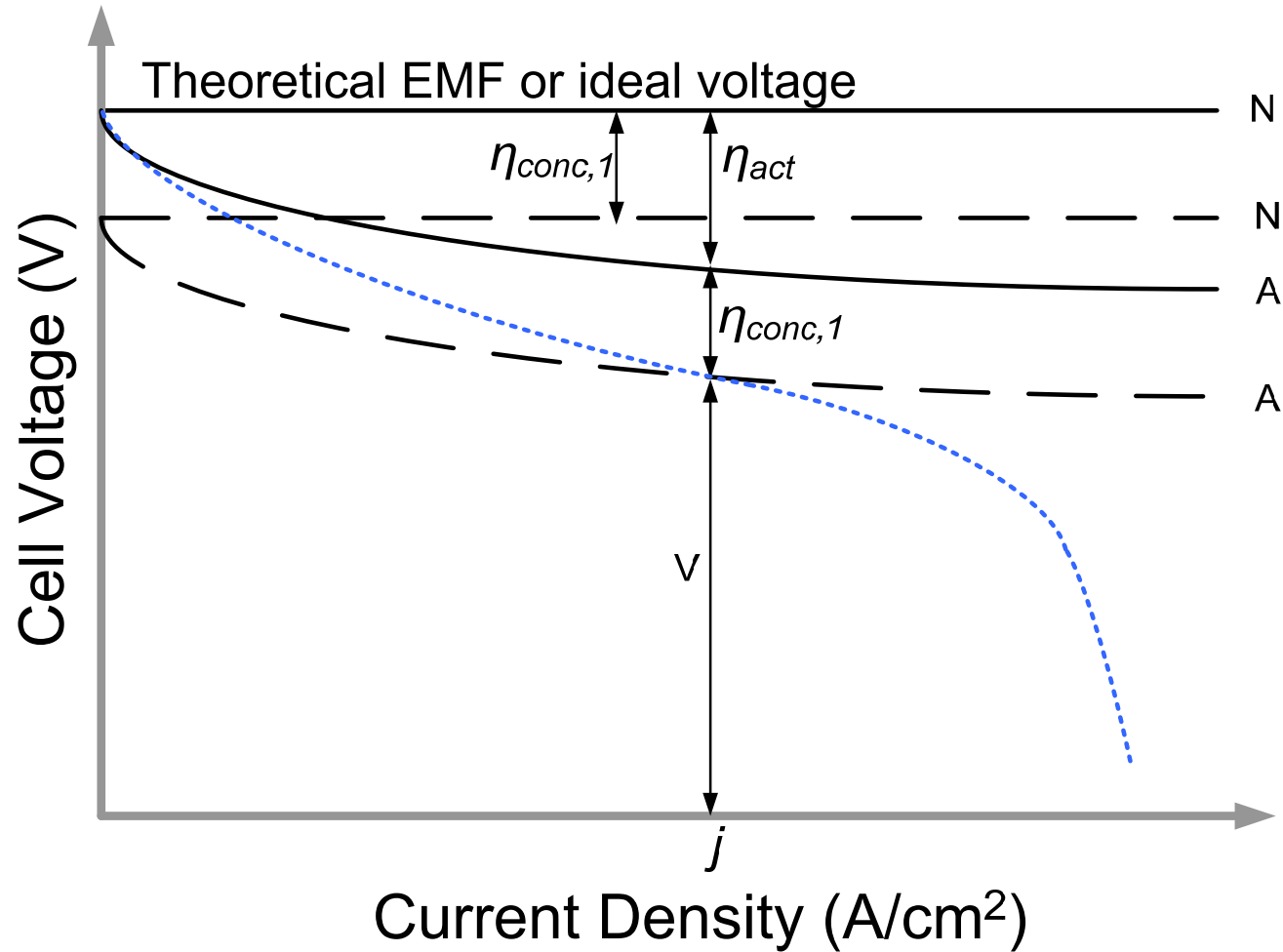
Adding two losses

$$\eta_{conc} = \frac{RT}{nF} \ln \frac{j_L}{j_L - j} + \frac{RT}{\alpha nF} \ln \frac{j_L}{j_L - j}$$
$$\eta_{conc} = \left(\frac{RT}{nF}\right) \left(1 + \frac{1}{\alpha}\right) \ln \frac{j_L}{j_L - j}$$



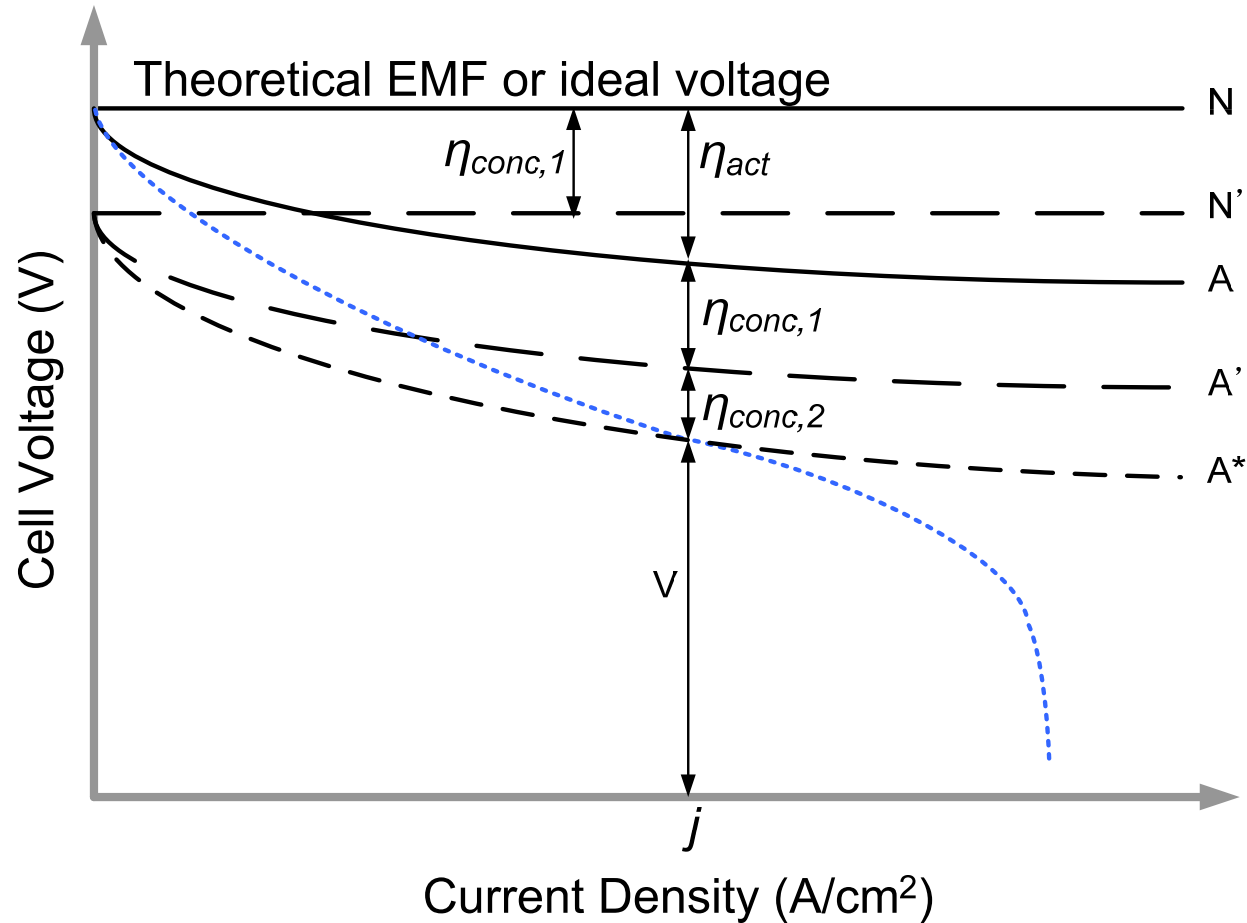
$$\eta_{conc} = c \ln \frac{j_L}{j_L - j}$$

Pictorial View



$$E = E^0 - \frac{RT}{nF} \ln \frac{\prod a_{PRODUCTS}^{v_i}}{\prod a_{REACTANTS}^{v_i}}$$

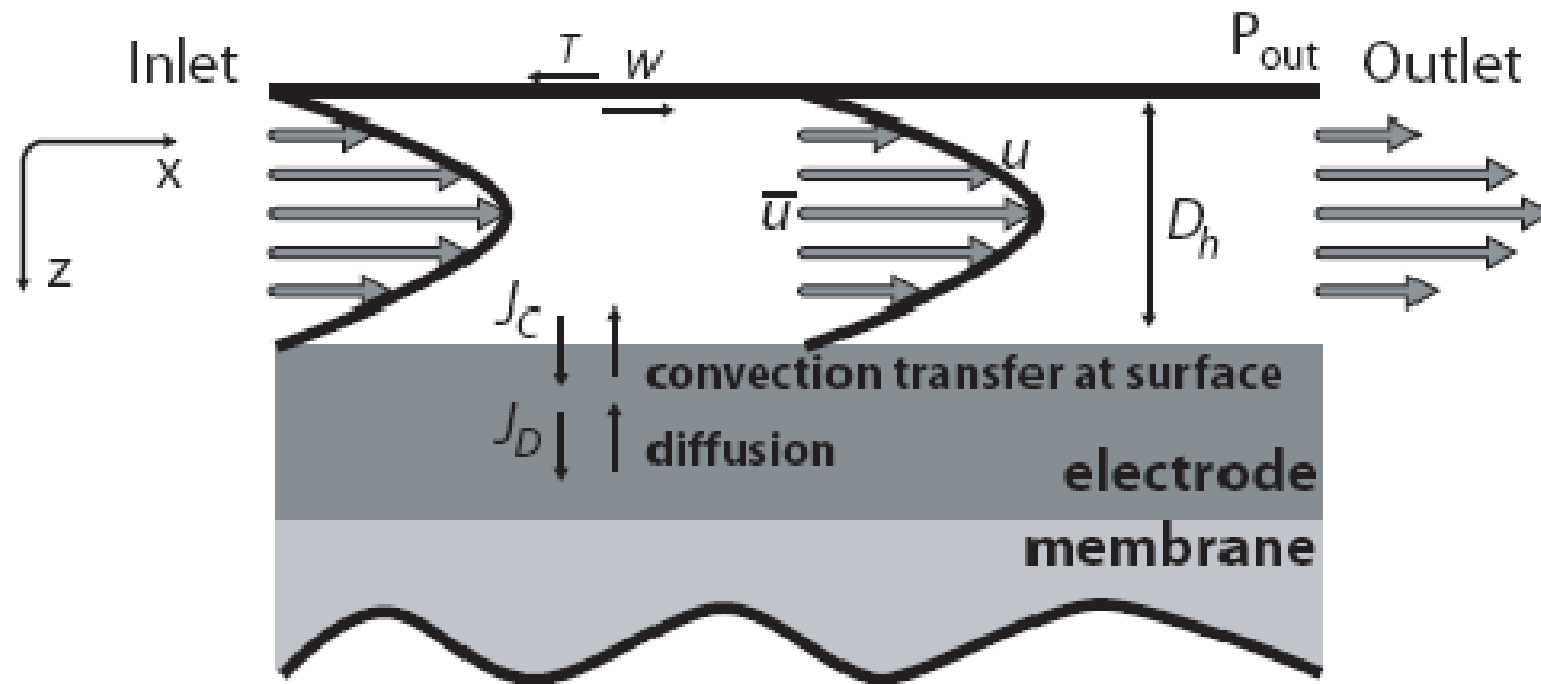
Pictorial View



$$E = E^0 - \frac{RT}{nF} \ln \frac{\prod a_{PRODUCTS}^{v_i}}{\prod a_{REACTANTS}^{v_i}}$$

$$j = j_0 \left(\frac{c_R^*}{c_R^{0*}} e^{\left(\frac{\alpha n F \eta_{act}}{RT} \right)} \right)$$

Convection



$$\tau_{xy} = 2\mu\dot{\epsilon}_{xy} = 2\mu \cdot \frac{1}{2} \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right)$$

Viscosity

Temperature effect

$$\frac{\mu}{\mu_0} \approx \left(\frac{T}{T_0}\right)^n \quad \text{or}$$

$$\frac{\mu}{\mu_0} \approx \left(\frac{T}{T_0}\right)^{1.5} \frac{T_0 + S}{T + S}$$

Gas	$\mu_0(10^{-6}(\text{kg}/\text{m}\cdot\text{s}))$	$T_0(\text{K})$	n	S
Air	17.16	273	0.666	111
CO ₂	13.7	273	0.79	222
CO	16.57	273	0.71	136
N ₂	16.63	273	0.67	107
O ₂	19.19	273	0.69	139
H ₂	8.411	273	0.68	97
H ₂ O(vapor)	11.2	350	1.15	1064

Mixture

$$\mu_{mix} = \sum_{i=1}^N \frac{x_i \mu_i}{\sum_{j=1}^N x_j \Phi_{ij}}$$

$$\Phi_{ij} = \frac{1}{\sqrt{8}} \left(1 + \frac{M_i}{M_j}\right)^{-1/2} \left[1 + \left(\frac{\mu_i}{\mu_j}\right)^{1/2} \left(\frac{M_i}{M_j}\right)^{1/4}\right]^2$$

Viscosity: Example

Example 5.1 Consider a fuel cell operating at 80°C . In the cathode, humidified air at 1 atm is supplied with a water vapor mole fraction of 0.2. If the fuel cell employs circular channels with a diameter of 1 mm, find the maximum tolerable air velocity that still ensures laminar flow.

$$\mu_{N_2}|_{80^\circ\text{C}} = \mu_0 \left(\frac{T}{T_0}\right)^n = 16.63 \left(\frac{353.15}{273}\right)^{0.67} = 19.76 \times 10^{-6} \text{ kg/m} \cdot \text{s} \quad (5.37)$$

Similarly, we can obtain $\mu_{O_2}|_{80^\circ\text{C}} = 22.92 \times 10^{-6} \text{ kg/m} \cdot \text{s}$ and $\mu_{H_2O}|_{80^\circ\text{C}} = 11.32 \times 10^{-6} \text{ kg/m} \cdot \text{s}$.

Species	Mole fraction, x_i	Molecular Weight, M_i	Viscosity, $\mu_i(10^{-6} \text{ kg/m} \cdot \text{s})$
1. N_2	$0.8 \times 0.79 = 0.632$	28.02	19.76
2. O_2	$0.8 \times 0.21 = 0.168$	32.00	22.92
3. H_2O	0.200	18.02	11.32

Viscosity: Example

Species i	Species j	M_i/M_j	μ_i/μ_j	Φ_{ij}	$x_j\Phi_{ij}$	$\sum_{j=1}^3 x_j\Phi_{ij}$
1. N ₂	1. N ₂	1.000	1.000	1.000	0.632	1.059
	2. O ₂	0.876	0.862	0.930	0.156	
	3. H ₂ O	1.555	1.746	1.356	0.271	
2. O ₂	1. N ₂	1.142	1.160	1.079	0.682	1.146
	2. O ₂	1.000	1.000	1.000	0.168	
	3. H ₂ O	1.776	2.025	1.482	0.296	
3. H ₂ O	1. N ₂	0.643	0.573	0.776	0.491	0.814
	2. O ₂	0.563	0.494	0.732	0.123	
	3. H ₂ O	1.000	1.000	1.000	0.200	

$$\begin{aligned} \mu_{mix} &= \left(\frac{0.632 \times 19.76}{1.059} + \frac{0.168 \times 22.92}{1.146} + \frac{0.200 \times 11.32}{0.814} \right) \times 10^{-6} \\ &= 17.93 \times 10^{-6} \text{ kg/m} \cdot \text{s} \end{aligned}$$

Viscosity: Example

$$M_{mix} = \sum_{i=1}^N x_i M_i = 0.632 \times 28.02 + 0.168 \times 32.00 + 0.200 \times 18.02 = 26.69 \text{ g/mol}$$

$$\rho = \frac{p}{\frac{R}{M_{mix}}} = \frac{101325 \text{ Pa}}{\frac{8.314 \text{ J/mol}\cdot\text{K}}{0.02669 \text{ kg/mol}} (273.15 + 80) \text{ T}} = 0.921 \text{ kg/m}^3$$

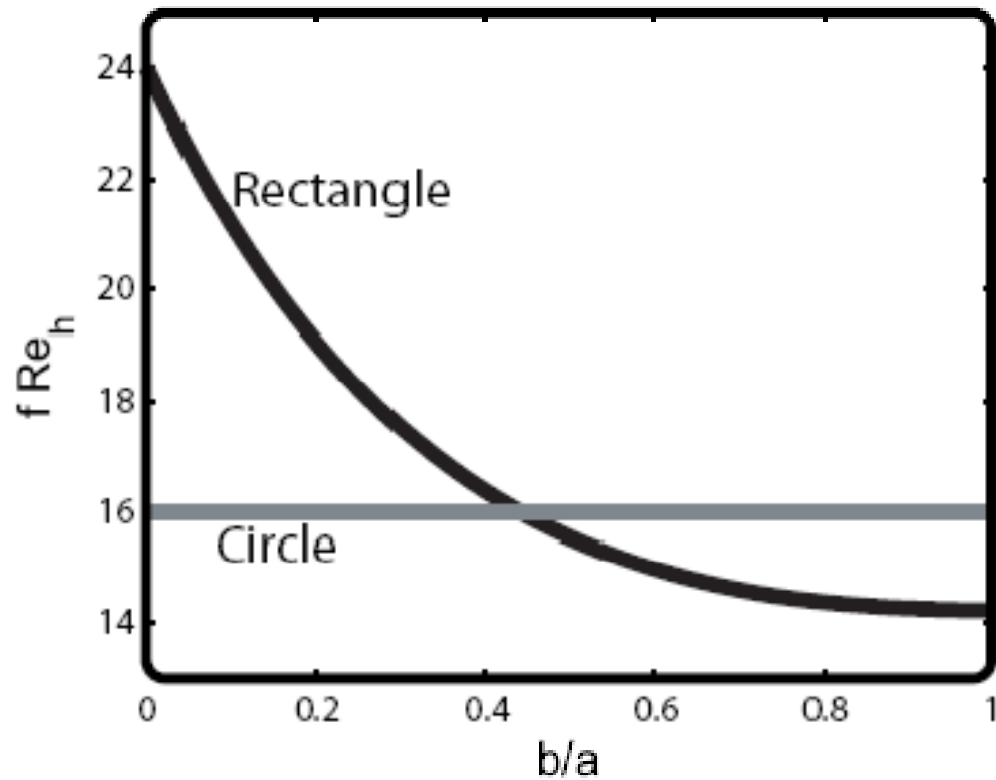
Roughly, laminar flow holds for $Re \sim 2000$, thus:

$$V_{max} = \frac{Re^{max} \mu_{mix}}{\rho L} = \frac{2000 \times (17.93 \times 10^{-6} \text{ kg/m}\cdot\text{s})}{(0.921 \text{ kg/m}^3) \times (0.001 \text{ m})} = 38.03 \text{ m/s} \quad (5.39)$$

This is very fast flow considering the channel is only 1 mm in diameter.

In general, flow in fuel cell is laminar.

Pressure Drop In Flow Channels



$$\frac{dp}{dx} = \frac{4}{D} \bar{\tau}_w$$

$$f = \frac{\bar{\tau}_w}{1/2 \rho \bar{u}^2}$$


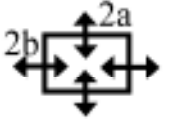

$$Re_h = \frac{\rho \bar{u} D_h}{\mu}$$

$$D_h = \frac{4A}{P} = \frac{4 \times \text{cross section area}}{\text{perimeter}}$$

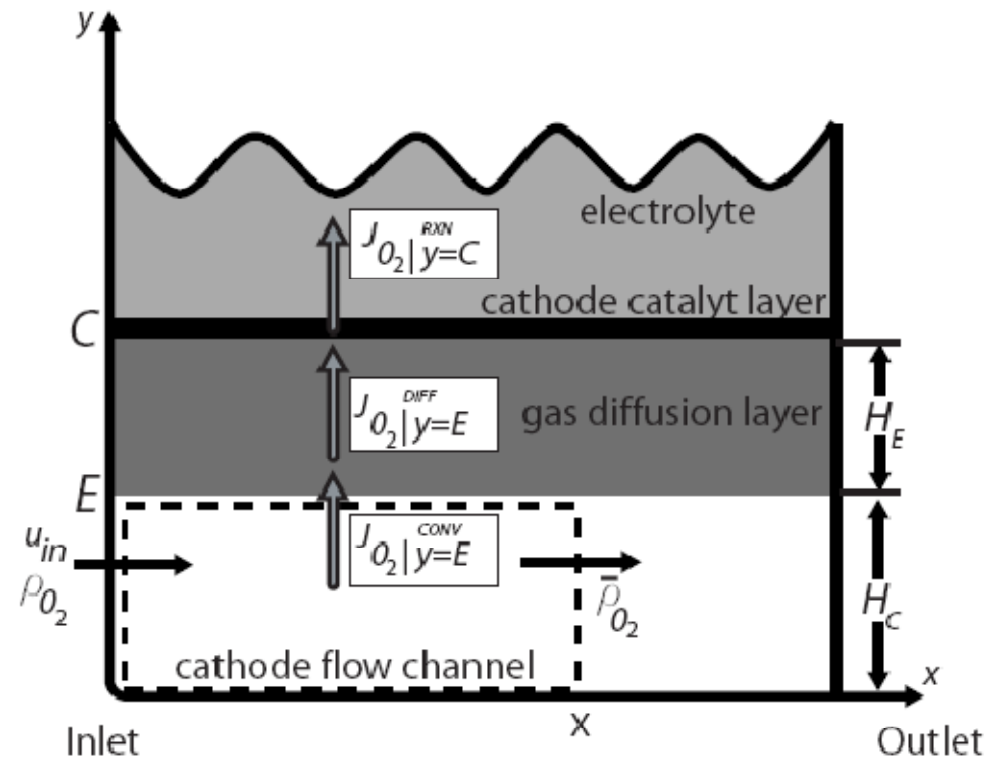
Convective Mass Transport

$$J_{C,i} = h_m (\rho_{i,s} - \bar{\rho}_i)$$

$$h_m = Sh \frac{D_{ij}}{D_h}$$

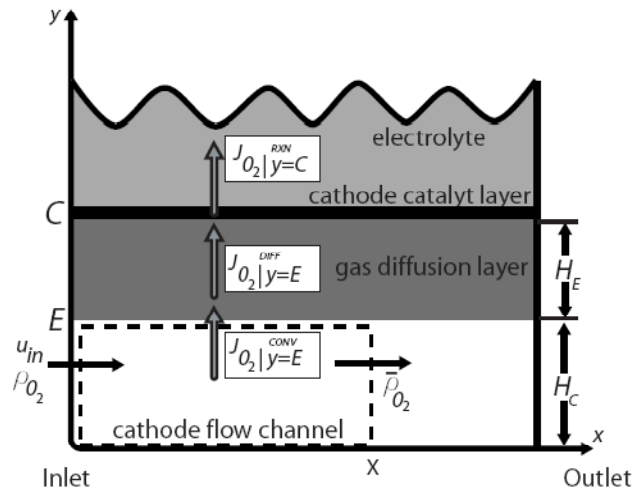
Cross section	α^*								
	0.2	0.4	0.7	1.0	2.0	2.5	5.0	10.0	
	Sh_D	4.36							
	Sh_F	3.66							
	Sh_D	4.80	3.67	3.08	2.97	3.38	3.67	4.80	5.86
	Sh_F	5.74	4.47	3.75	3.61	4.12	4.47	5.74	6.79
	Sh_D	0.83	1.42	2.02	2.44	3.19	3.39	3.91	4.27
	Sh_F	0.96	1.60	2.26	2.71	3.54	3.78	4.41	4.85

Convective Mass Transport in PEMFC



1. The catalyst layer is infinitely thin.¹
2. Water exists only in the vapor form.
3. Diffusive mass transport dominates in the diffusion layer. Furthermore, only y-direction diffusion is considered.
4. Convection dominates in the flow channel.
5. Flow velocity in the channel is constant.

Convective Mass Transport in PEMFC



$$\hat{J}_{O_2}|_{x=X,y=C}^{rxn} = M_{O_2} \frac{j(X)}{4F}$$

$$\hat{J}_{O_2}|_{x=X,y=E}^{diff} = -D_{O_2}^{eff} \frac{\rho_{O_2}|_{x=X,y=C} - \rho_{O_2}|_{x=X,y=E}}{H_E}$$

$$\hat{J}_{O_2}|_{x=X,y=E}^{conv} = -h_m (\rho_{O_2}|_{x=X,y=E} - \bar{\rho}_{O_2}|_{x=X,y=channel})$$

$$\hat{J}_{O_2}|_{x=X,y=C}^{rxn} = \hat{J}_{O_2}|_{x=X,y=E}^{diff} = \hat{J}_{O_2}|_{x=X,y=E}^{conv}$$

$$\hat{J}_{O_2}|_{x=X,y=E}^{conv} = M_{O_2} \frac{j(X)}{4F}$$

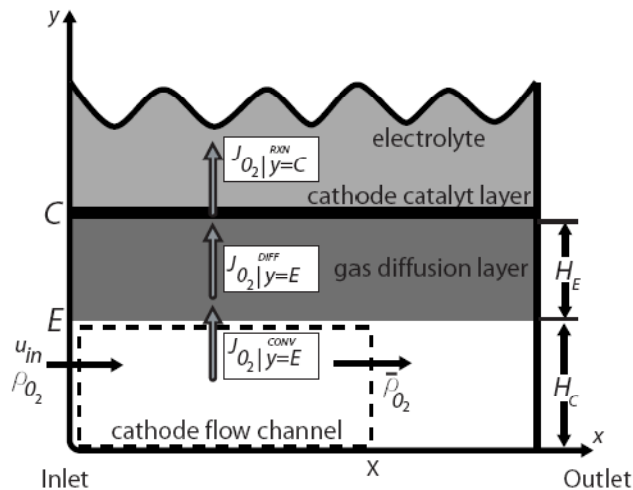
$$\rho_{O_2}|_{x=X,y=C} = \rho_{O_2}|_{x=X,y=E} - M_{O_2} \frac{j(X)}{4F} \frac{H_E}{D_{O_2}^{eff}}$$

$$\rho_{O_2}|_{x=X,y=E} = \bar{\rho}_{O_2}|_{x=X,y=channel} - M_{O_2} \frac{j(X)}{4F} \frac{1}{h_m}$$

Convective Mass Transport in PEMFC

$$u_{in} H_C \bar{\rho}_{O_2} |_{x=0, y=channel} - u_{in} H_C \bar{\rho}_{O_2} |_{x=X, y=channel} = \int_0^X \left(\hat{J}_{O_2} |_{y=E}^{conv} \right) dx \quad (5.6)$$

Amount of gas entering from left
Amount of gas leaving from right
Amount of gas leaving out the top

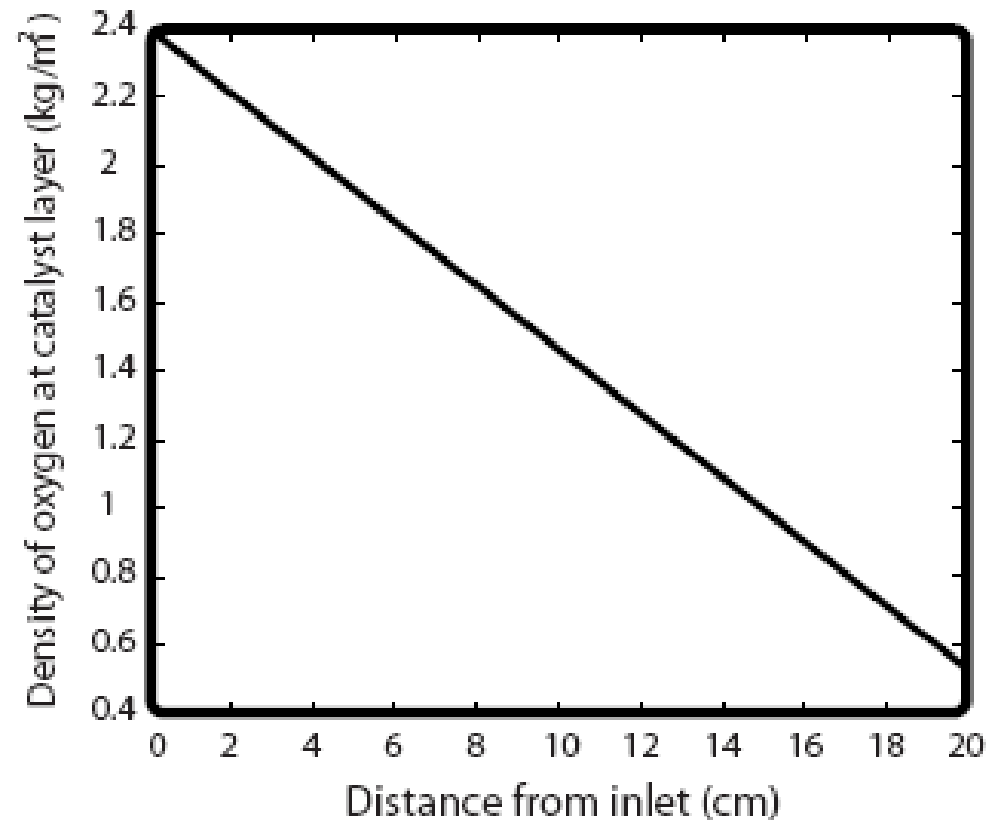


$$\int_0^X \left(\hat{J}_{O_2} |_{y=E}^{conv} \right) dx = \int_0^X \frac{M_{O_2} j(x)}{4F} dx$$

$$\rho_{O_2} |_{x=X, y=C} = \bar{\rho}_{O_2} |_{x=0, y=channel} - \frac{M_{O_2}}{4F} \left(\frac{j(X)}{h_m} + \frac{H_E j(X)}{D_{O_2}^{eff}} + \int_0^X \frac{j(x)}{u_{in} H_C} dx \right)$$

$$\rho_{O_2} |_{x=X, y=C} = \bar{\rho}_{O_2} |_{x=0, y=channel} - M_{O_2} \frac{j}{4F} \left(\frac{1}{h_m} + \frac{H_E}{D_{O_2}^{eff}} + \frac{X}{u_{in} H_C} \right)$$

Convective Mass Transport in PEMFC

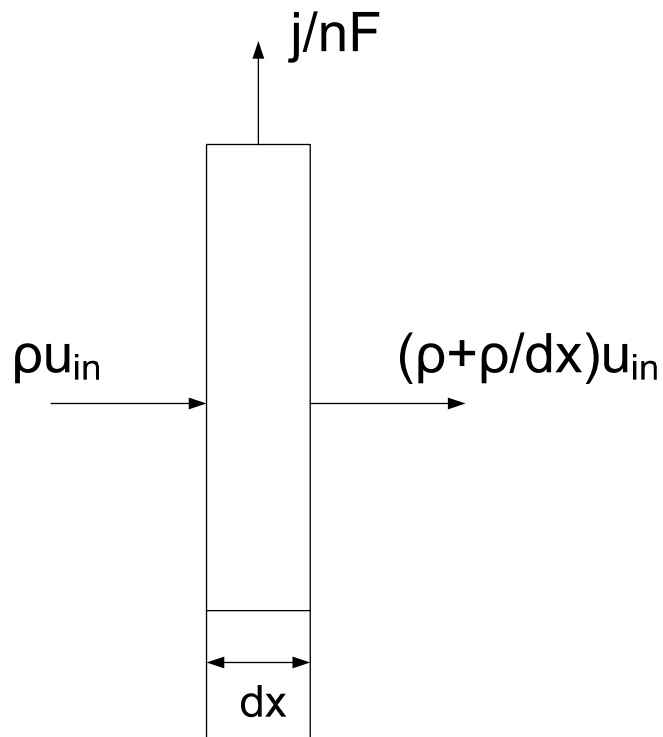


$$\rho_{O_2}|_{x=X,y=C} = \bar{\rho}_{O_2}|_{x=0,y=channel} - M_{O_2} \frac{j}{4F} \left(\frac{H_C}{Sh_F D_{O_2}} - \frac{H_E}{D_{O_2}^{eff}} + \frac{X}{u_{in} H_C} \right)$$

$$h_m = \frac{Sh_F D_{O_2}}{H_C} \quad N_{total} = u_{in} H_C = constant$$

A More Realistic Alternative Solution

$$\rho_{O_2}|_{x=X,y=C} = \bar{\rho}_{O_2}|_{x=0,y=channel} - \frac{M_{O_2}}{4F} \left(\frac{j(X)}{h_m} + \frac{H_E j(X)}{D_{O_2}^{eff}} + \int_0^X \frac{j(x)}{u_{in} H_C} dx \right)$$



$$u_{in}\rho - u_{in}\left(\rho + \frac{\rho}{dx}\right) = \frac{j(x)}{nF} dx$$

$$\frac{d\rho}{dx} = -\frac{j(x)}{u_{in}nF}$$

$$\frac{dC(x)}{dx} = -Bj(x)$$

A More Realistic Alternative Solution

If constant Voltage instead of constant current is assumed

$$j = j_0^0 \frac{c_R^*}{c_R^{0*}} e^{\alpha n F \eta / RT}$$

$$\frac{dc(x)}{dx} = -Bj(x) = -Bj_0^0 \frac{c(x)}{c^0} e^{\alpha n F \eta / RT} = ac(x)$$

$$c(x) = Ae^{-ax}$$

$$c(0) = c_{in} = A$$

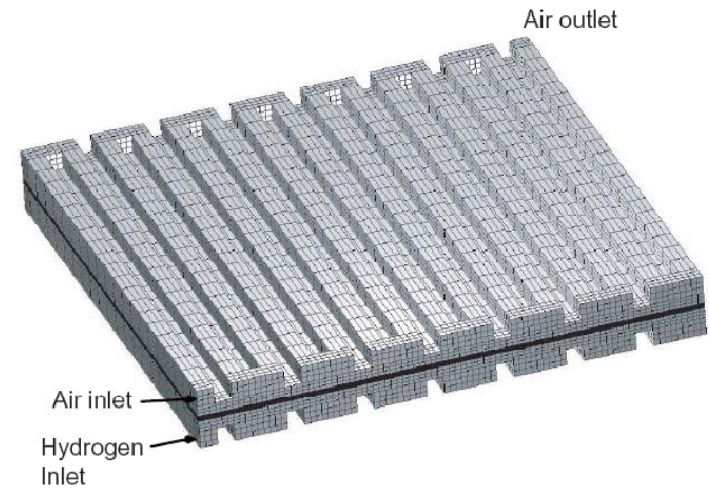
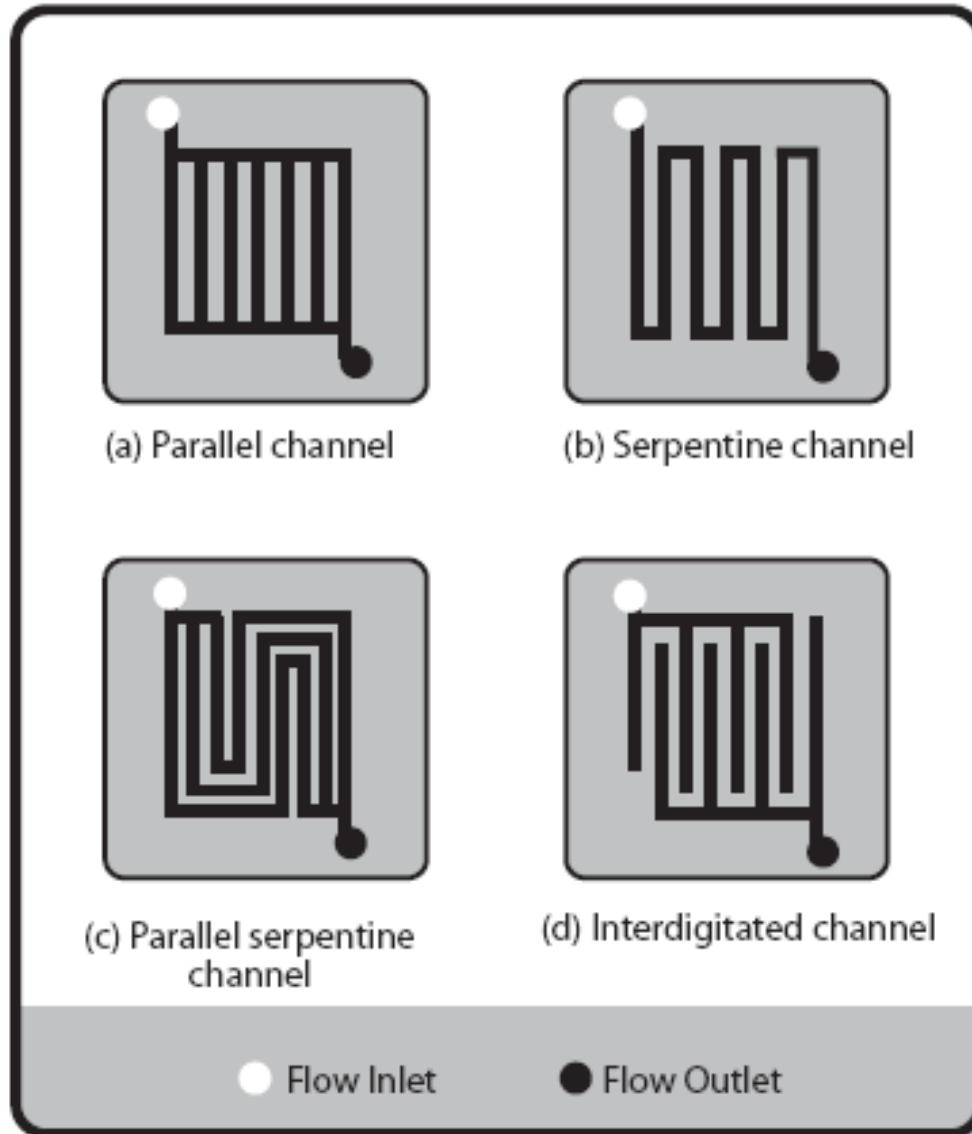
$$j(x) = Ke^{-ax}$$

- Current drop Exponentially
- Concentration also drop exponentially
- HW 5.10

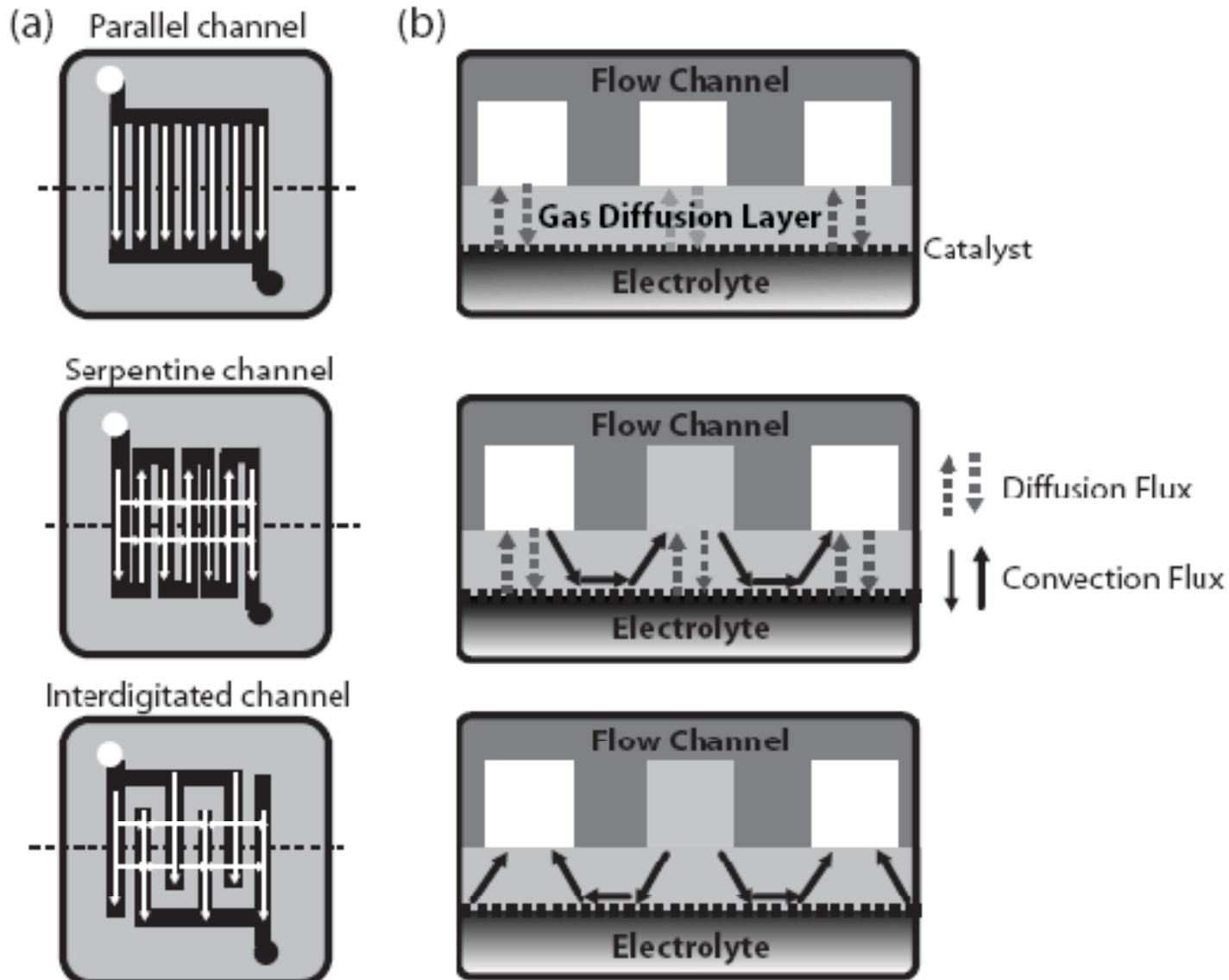
Flow Channel Design

- High electrical conductivity
- High corrosion resistance
- High chemical compatibility
- High thermal conductivity
- High gas tightness
- High mechanical strength
- Low weight and volume
- Ease of manufacturability
- Cost effectiveness

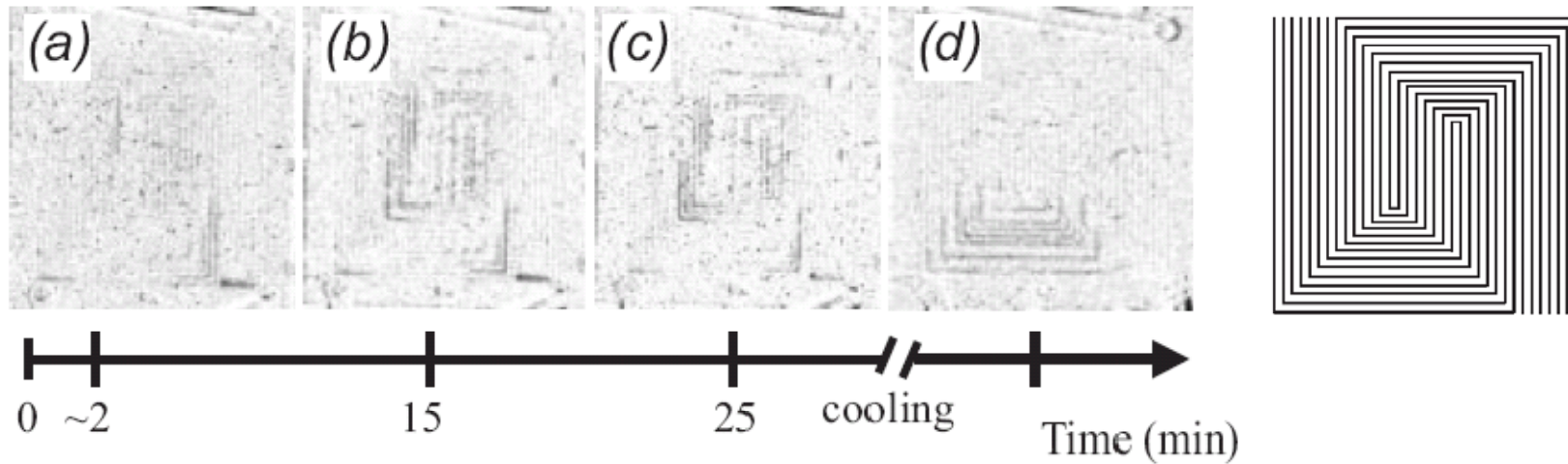
PEMFC Flow Channel Design



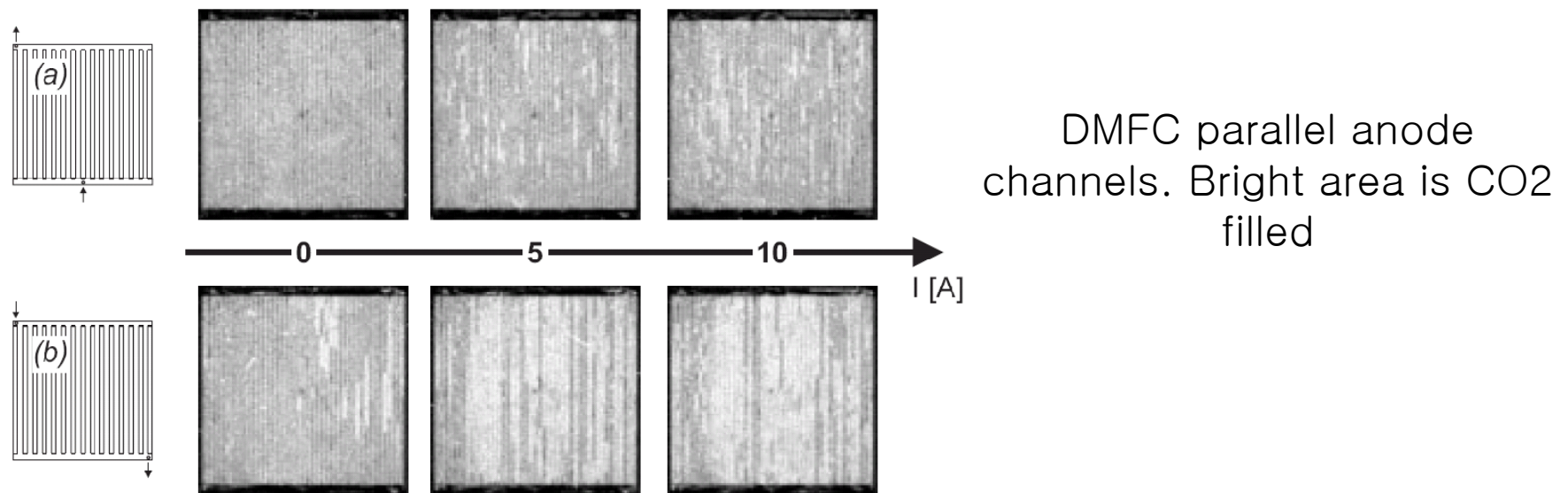
PEMFC Flow Channel Design



Flow Visualization (Neutron Radiography)



PEMFC serpentine cathode channels. Dark area is liquid filled.



Flow Visualization

