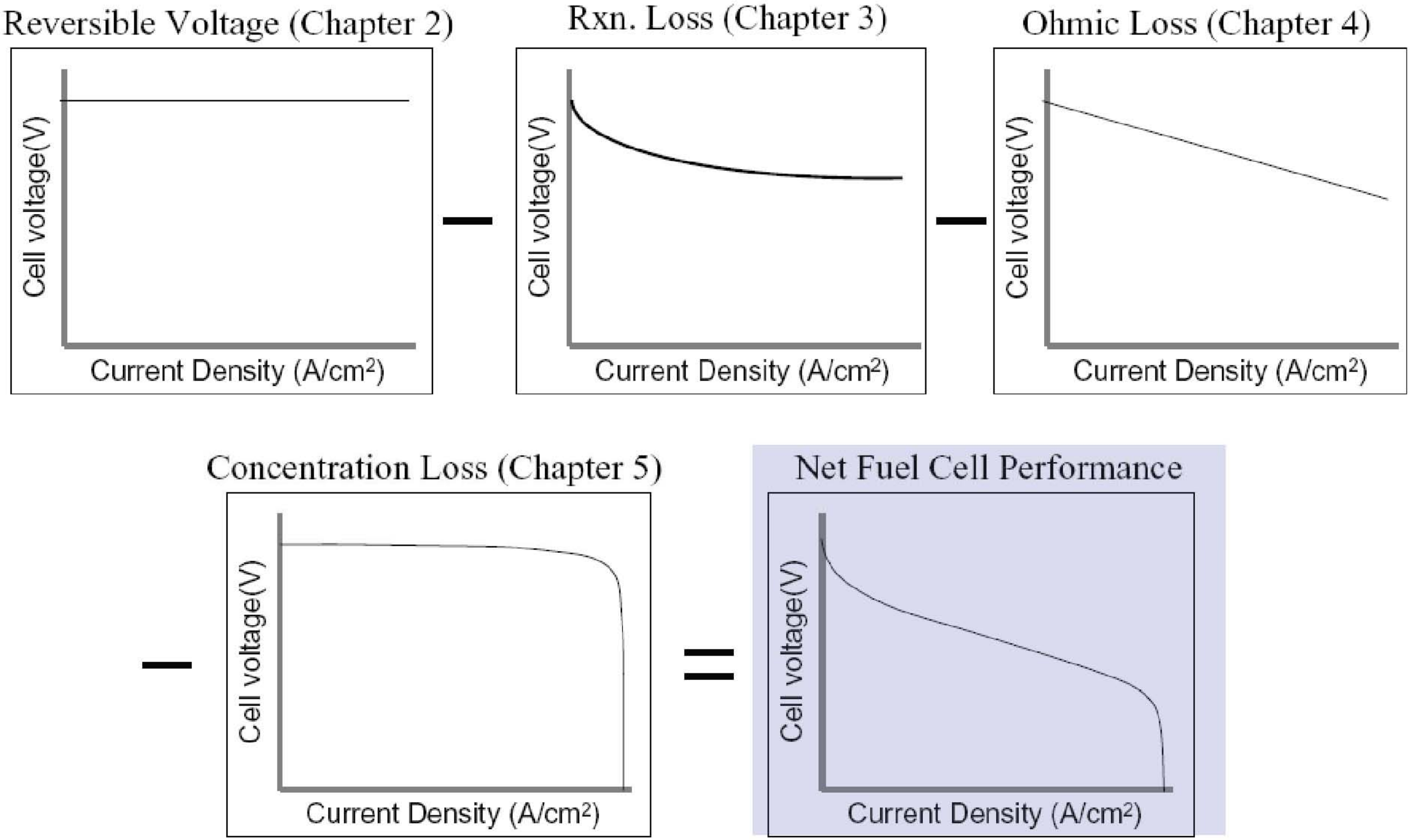
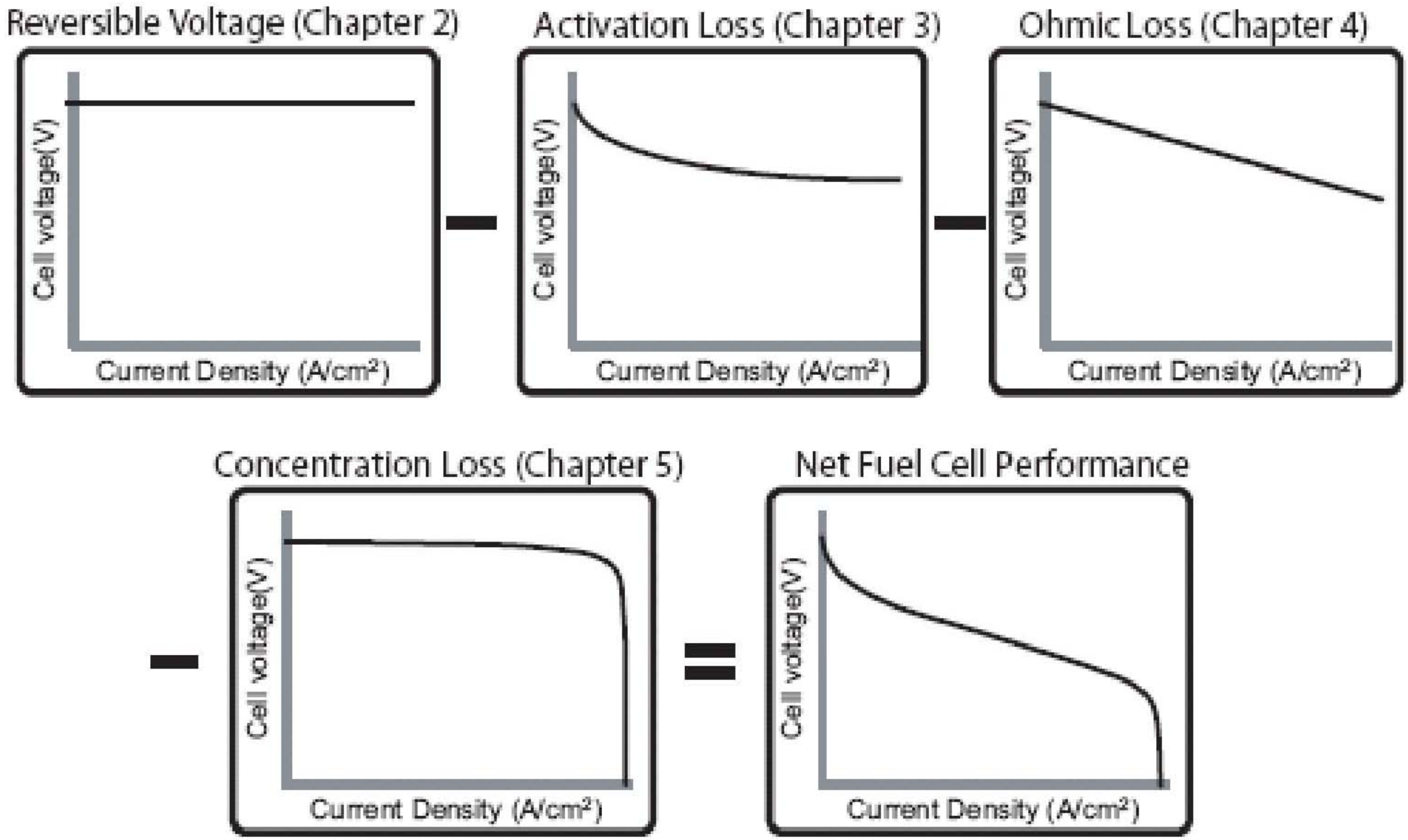
Losses in Fuel Cells



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

Fuel Cell Modeling

Basic Fuel Cell Model



$$V = E_{thermo} - (a_A + b_A \ln j) - (a_C + b_C \ln j) - (j\,ASR_{ohmic}) - \left(c \ln \frac{j_L}{j_L - j}\right)$$

Basic Fuel Cell Model

$$V = E_{thermo} - (a_A + b_A \ln j) - (a_C + b_C \ln j) - (j ASR_{ohmic}) - \left(c \ln \frac{j_L}{j_L - j} \right)$$

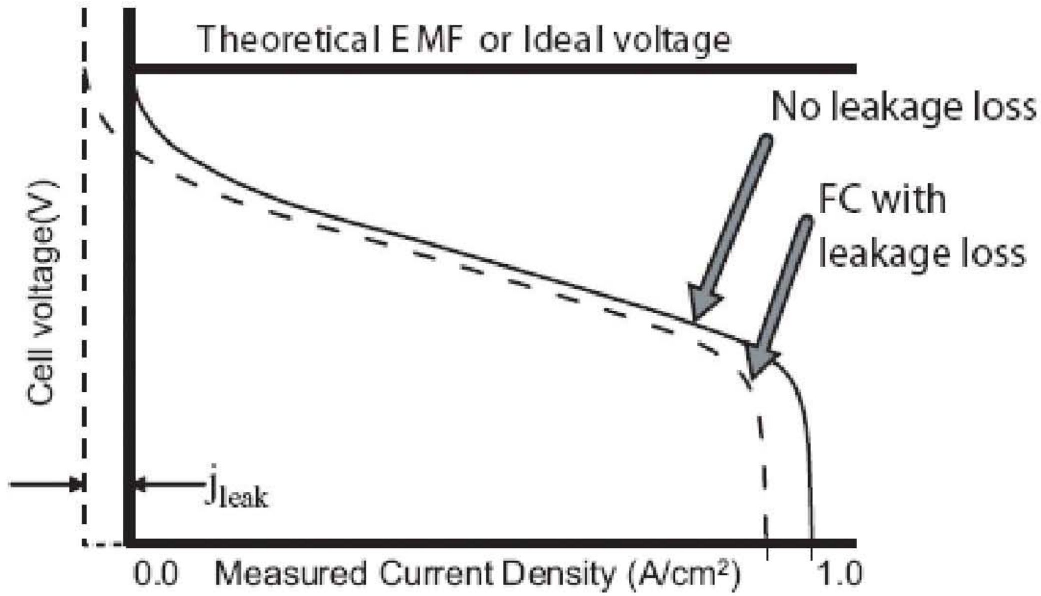
- $\eta_{act} = (a_A + b_A \ln j) + (a_C + b_C \ln j)$: The activation losses from both the anode (A) and the cathode (C) based on the natural logarithm form of the Tafel Equation (equation 3.41).

- $\eta_{ohmic} = j ASR_{ohmic}$: The ohmic resistance loss based on current density and area specific resistance (Equation 4.11).

- $\eta_{conc} = c \ln \frac{j_L}{j_L - j}$: The combined fuel cell concentration loss based on equation 5.25, where c is an empirical constant.

Only valid for $j >> j_0$

Leakage Current



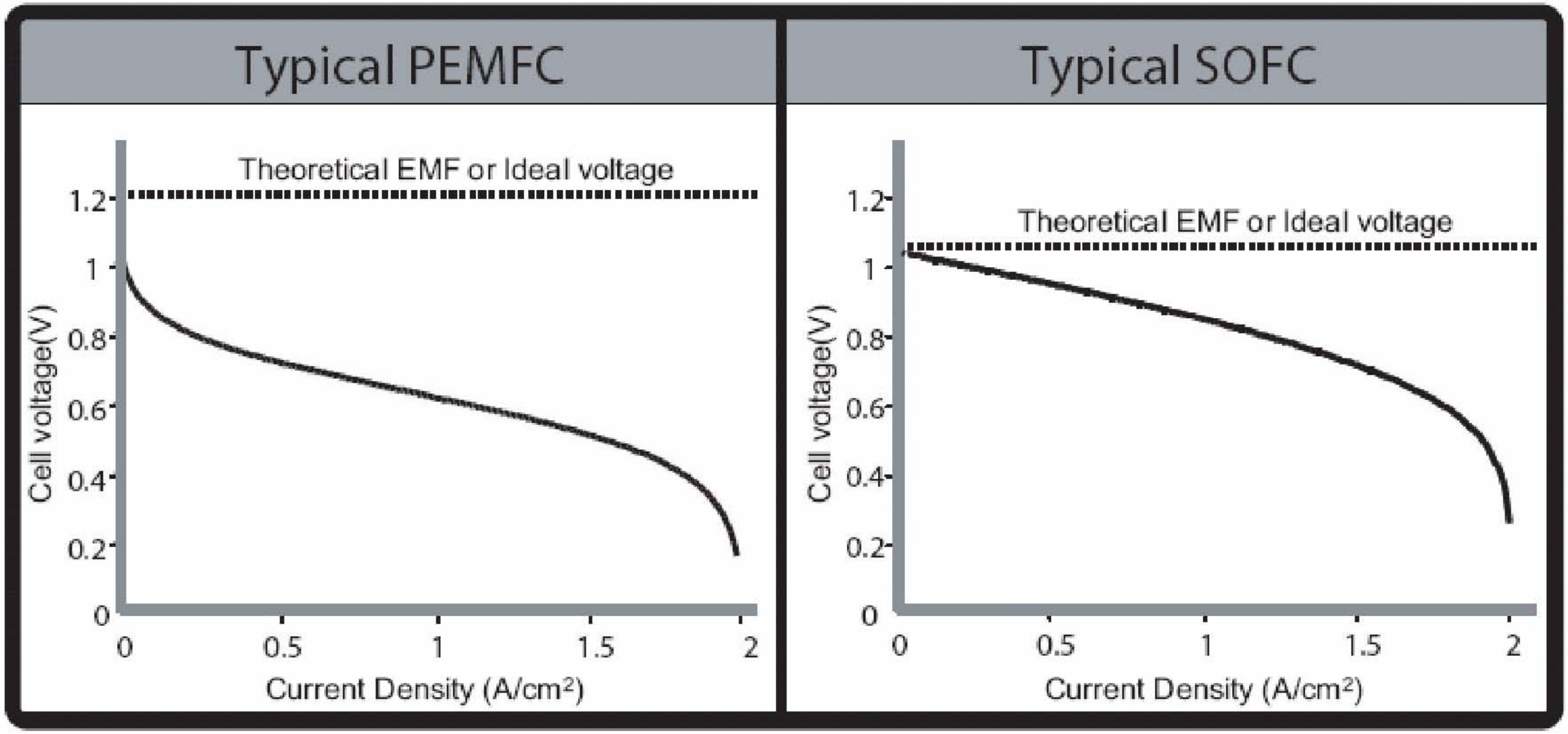
$$j_{gross} = j + j_{leak}$$

$$V = E_{thermo} - (a_A + b_A \ln(j + j_{leak})) - (a_C + b_C \ln(j + j_{leak})) \\ -(jASR_{ohmic}) - \left(c \ln \frac{j_L}{j_L - (j + j_{leak})}\right)$$

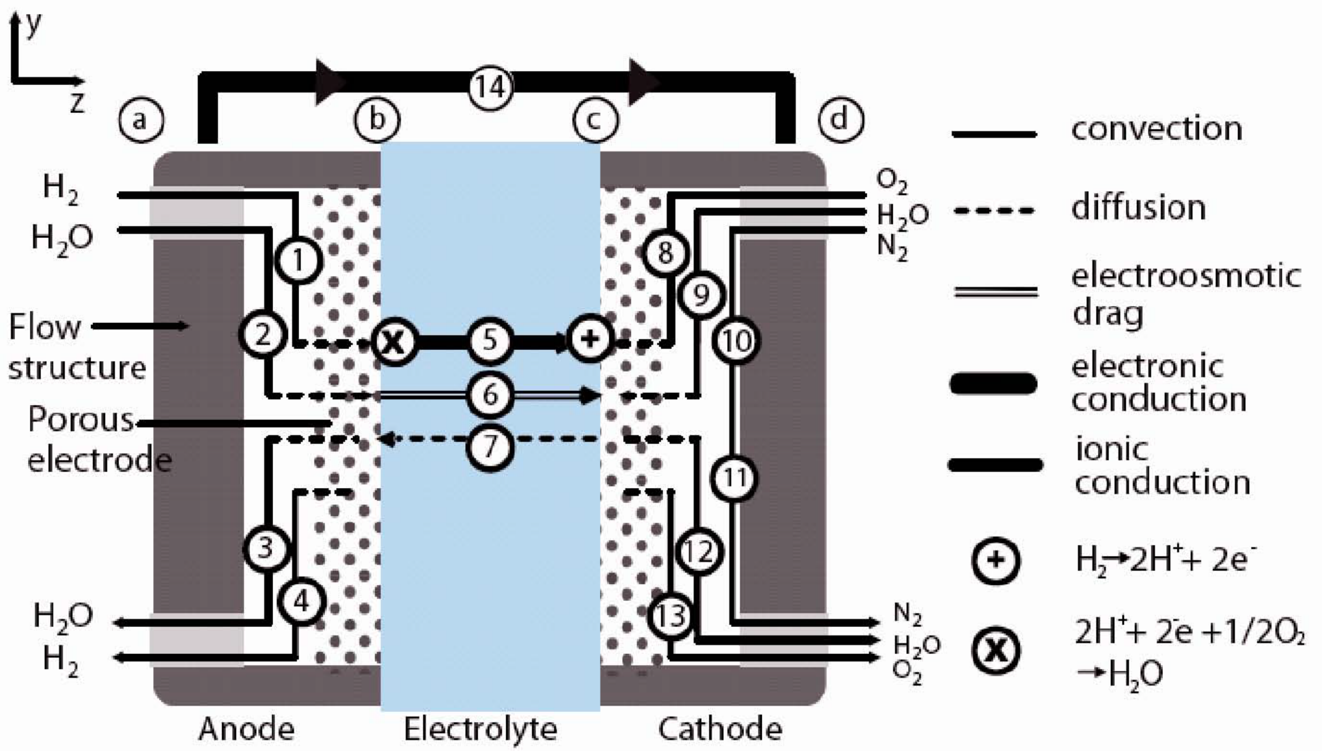
Typical Parameters

Parameter	Typical Value for PEMFC	Typical Value for SOFC
$Temperature$	350 K	1000 K
E_{thermo}	1.22 V	1.06 V
j_0 (H_2)	0.10 A/cm^2	10 A/cm^2
j_0 (O_2)	10^{-4} A/cm^2	0.10 A/cm^2
α (H_2)	0.50	0.50
α (O_2)	0.30	0.30
ASR_{ohmic}	0.01 Ωcm^2	0.04 Ωcm^2
j_{leak}	10^{-2} A/cm^2	10^{-2} A/cm^2
j_L	2 A/cm^2	2 A/cm^2
c	0.10 V	0.10 V

Typical High & Low Temperature Fuel Cells



1-D Fuel Cell Model: PEMFC

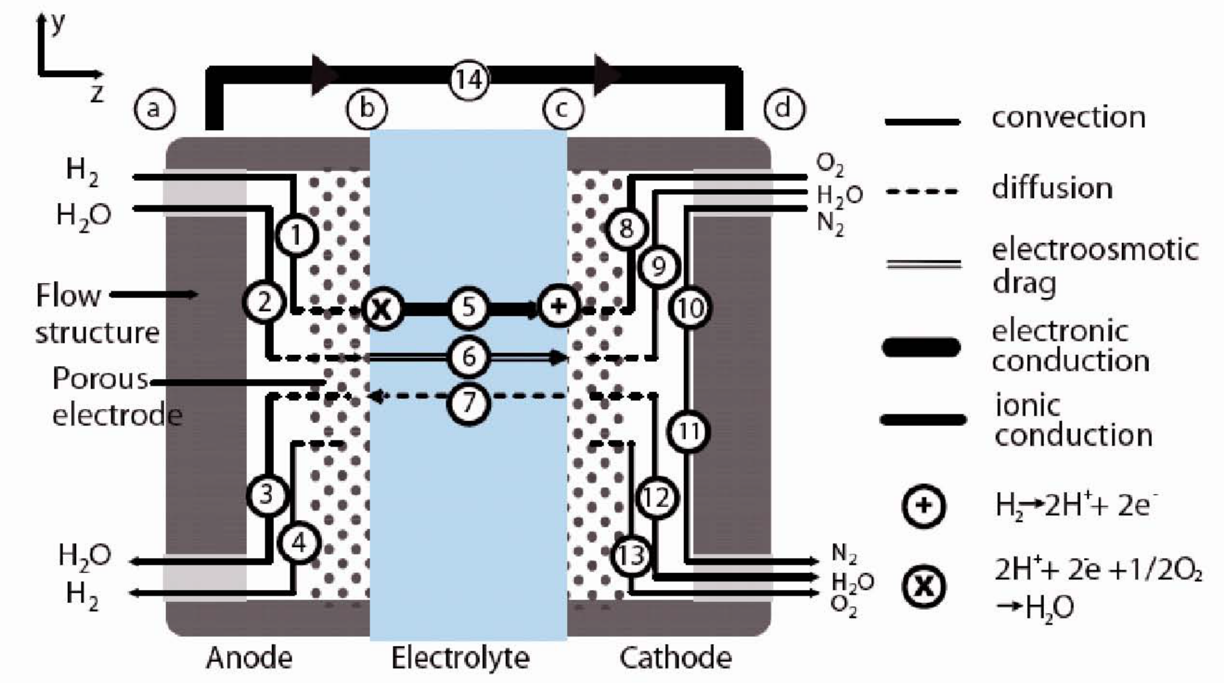


(a) In a PEMFC, water(H_2O) and proton(H^+) transport through the electrolyte.

$$flux\ 14 = flux\ 5 = flux\ 1 - flux\ 4 = flux\ 8 - flux\ 13$$

$$\frac{j}{2F} = \frac{J_{H+}}{2} = J_{H_2}^{A} = 2J_{O_2}^{C} = S_{H_2O}^{C}$$

1-D PEMFC Model: Water Flux



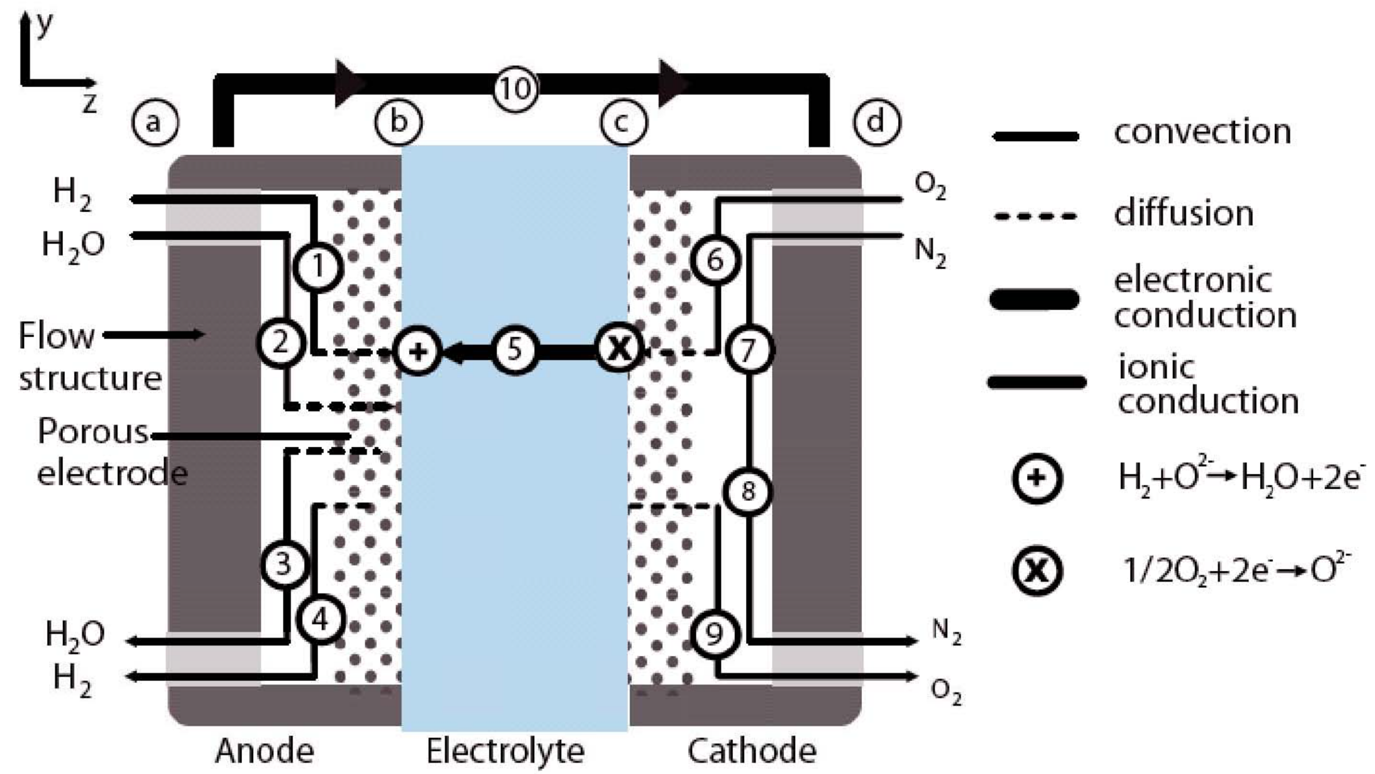
(a) In a PEMFC, water(H_2O) and proton(H^+) transport through the electrolyte.

$$\underbrace{flux\ 2 - flux\ 3}_{anode} = \underbrace{flux\ 6 - flux\ 7}_{membrane} = \underbrace{flux\ 12 - flux\ 9 - flux\ 5}_{cathode}$$

$$J^A_{H_2O} = J^M_{H_2O} = J^C_{H_2O} - \frac{j}{2F} \qquad \alpha = \frac{J^M_{H_2O}}{\frac{j}{2F}}$$

$$\frac{j}{2F} = \frac{J^M_{H+}}{2} = J^A_{H_2} = 2J^C_{O_2} = \frac{J^A_{H_2O}}{\alpha} = \frac{J^M_{H_2O}}{\alpha} = \frac{J^C_{H_2O}}{1+\alpha}1$$

1-D Fuel Cell Model: SOFC



(b) In a SOFC, oxygen ions(O^{2-}) transport through the electrolyte.

$$\frac{j}{2F} = J^{M}_{O^{2-}} = J^{A}_{H_2} = 2J^{C}_{O_2} = -J^{A}_{H_2O}$$

Full Model

Domains \ Phenomena		Convection	Diffusion	Conduction	Electrochemical Reaction
Anode	Flow Channels	(1) $\mathrm{H_2, H_2O_{(g)}, H_2O_{(l)}}$ (1) $H_2, H_2O_{(g)}$	(2) $\mathrm{H_2, H_2O_{(g)}, H_2O_{(l)}}$ (2) $H_2, H_2O_{(g)}$	(3) $\mathrm{e^-}$ (3) e^-	. .
	Electrode	(1) $\mathrm{H_2, H_2O_{(g)}, H_2O_{(l)}}$ (1) $H_2, H_2O_{(g)}$	(6) $\mathrm{H_2, H_2O_{(g)}, H_2O_{(l)}}$ $H_2, H_2O_{(g)}$	(3) $\mathrm{e^-}$ (3)(5) e^-, O^{2-}	. (5) $H_2 + O^{2-} \rightarrow H_2O + 2e^-$
	Catalyst	(1) $\mathrm{H_2, H_2O_{(g)}, H_2O_{(l)}}$ (1) $H_2, H_2O_{(g)}$	(5) $\mathrm{H_2, H_2O_{(g)}, H_2O_{(l)}}$ (5) $H_2, H_2O_{(g)}$	(3)(5) $\mathrm{e^-, H^+}$ (3)(5) e^-, O^{2-}	(4) $\mathrm{H_2 \rightarrow 2H^+ + 2e^-}$ $H_2 + O^{2-} \rightarrow H_2O + 2e^-$
Electrolyte		. .	(6) $\mathrm{H_2O_{(l)}}$.	(6) $\mathrm{H^+, H_2O_{(l)}}$ [a] O^{2-}	. .
Cathode	Catalyst	(1) $\mathrm{N_2, O_2, H_2O_{(g)}, H_2O_{(l)}}$ (1) N_2, O_2	(5) $\mathrm{N_2, O_2, H_2O_{(g)}, H_2O_{(l)}}$ (5) N_2, O_2	(3)(5) $\mathrm{e^-, H^+}$ (3)(5) e^-, O^{2-}	(6) $\mathrm{2H^+ + \frac{1}{2}O_2 + 2e^- \rightarrow H_2O_{(l)}}$ $\frac{1}{2}O_2 + 2e^- \rightarrow O^{2-}$
	Electrode	(1) $\mathrm{N_2, O_2, H_2O_{(g)}, H_2O_{(l)}}$ (1) N_2, O_2	(6) $\mathrm{N_2, O_2, H_2O_{(g)}, H_2O_{(l)}}$ N_2, O_2	(3) $\mathrm{e^-}$ (3)(5) e^-, O^{2-}	. (5) $\frac{1}{2}O_2 + 2e^- \rightarrow O^{2-}$
	Flow Channels	(1) $\mathrm{N_2, O_2, H_2O_{(g)}}$ (1) N_2, O_2	(2) $\mathrm{N_2, O_2, H_2O_{(g)}, H_2O_{(l)}}$ (2) N_2, O_2	(3) $\mathrm{e^-}$ (3) e^-	. .

Table 6.2: Description of a full PEMFC (or SOFC in italics) model. Six key assumptions, numbered (1-6) in parentheses, lead to the simplified model shown in table 6.3.

[a] To be precise, this water transport phenomenon is due to electro-osmotic drag (See chapter 4). For convenience, it has been categorized as conduction due to its close relationship with proton conduction.

Simplifying Model

Domains \ Phenomena		Convection	Diffusion	Conduction	Electrochemical Reaction
Anode	Flow Channels	(1)$H_2, H_2O_{(g)}, H_2O_{(l)}$ (1)*$H_2, H_2O_{(g)}$*	(2)$H_2, H_2O_{(g)}, H_2O_{(l)}$ (2)*$H_2, H_2O_{(g)}$*	(3)e^- (3)*e^-*	. .
	Electrode	(1)$H_2, H_2O_{(g)}, H_2O_{(l)}$ (1)*$H_2, H_2O_{(g)}$*	(6)$H_2, H_2O_{(g)}, H_2O_{(l)}$ *$H_2, H_2O_{(g)}$*	(3)e^- (3)(5)*e^-, O^{2-}*	. (5)*$H_2 + O^{2-} \rightarrow H_2O + 2e^-$*
	Catalyst	(1)$H_2, H_2O_{(g)}, H_2O_{(l)}$ (1)*$H_2, H_2O_{(g)}$*	(5)$H_2, H_2O_{(g)}, H_2O_{(l)}$ (5)*$H_2, H_2O_{(g)}$*	(3)(5)e^-, H^+ (3)(5)*e^-, O^{2-}*	(4)$H_2 \rightarrow 2H^+ + 2e^-$ *$H_2 + O^{2-} \rightarrow H_2O + 2e^-$*
Electrolyte		. .	(6)$H_2O_{(l)}$.	(6)$H^+, H_2O_{(l)}$[a] *O^{2-}*	. .
Cathode	Catalyst	(1)$N_2, O_2, H_2O_{(g)}, H_2O_{(l)}$ (1)*N_2, O_2*	(5)$N_2, O_2, H_2O_{(g)}, H_2O_{(l)}$ (5)*N_2, O_2*	(3)(5)e^-, H^+ (3)(5)*e^-, O^{2-}*	(6)$2H^+ + \frac{1}{2}O_2 + 2e^- \rightarrow H_2O_{(l)}$ *$\frac{1}{2}O_2 + 2e^- \rightarrow O^{2-}$*
	Electrode	(1)$N_2, O_2, H_2O_{(g)}, H_2O_{(l)}$ (1)*N_2, O_2*	(6)$N_2, O_2, H_2O_{(g)}, H_2O_{(l)}$ *N_2, O_2*	(3)e^- (3)(5)*e^-, O^{2-}*	. (5)*$\frac{1}{2}O_2 + 2e^- \rightarrow O^{2-}$*
	Flow Channels	(1)$N_2, O_2, H_2O_{(g)}$ (1)*N_2, O_2*	(2)$N_2, O_2, H_2O_{(g)}, H_2O_{(l)}$ (2)*N_2, O_2*	(3)e^- (3)*e^-*	. .

Table 6.2: Description of a full PEMFC (or SOFC in italics) model. Six key assumptions, numbered (1-6) in parentheses, lead to the simplified model shown in table 6.3.

[a] To be precise, this water transport phenomenon is due to electro-osmotic drag (See chapter 4). For convenience, it has been categorized as conduction due to its close relationship with proton conduction.

1. Ignore convection in flow channels

Simplifying Model

Domains		Convection	Diffusion	Conduction	Electrochemical Reaction
Anode	Flow Channels	(1) $H_2, H_2O_{(g)}, H_2O_{(l)}$ (1) $\mathit{H_2, H_2O_{(g)}}$	(2) $H_2, H_2O_{(g)}, H_2O_{(l)}$ (2) $\mathit{H_2, H_2O_{(g)}}$	(3) e^- (3) $\mathit{e^-}$	. .
	Electrode	(1) $H_2, H_2O_{(g)}, H_2O_{(l)}$ (1) $\mathit{H_2, H_2O_{(g)}}$	(6) $H_2, H_2O_{(g)}, H_2O_{(l)}$ $\mathit{H_2, H_2O_{(g)}}$	(3) e^- (3)(5) $\mathit{e^-, O^{2-}}$	. (5) $\mathit{H_2 + O^{2-} \rightarrow H_2O + 2e^-}$
	Catalyst	(1) $H_2, H_2O_{(g)}, H_2O_{(l)}$ (1) $\mathit{H_2, H_2O_{(g)}}$	(5) $H_2, H_2O_{(g)}, H_2O_{(l)}$ (5) $\mathit{H_2, H_2O_{(g)}}$	(3)(5) e^-, H^+ (3)(5) $\mathit{e^-, O^{2-}}$	(4) $H_2 \rightarrow 2H^+ + 2e^-$ $\mathit{H_2 + O^{2-} \rightarrow H_2O + 2e^-}$
Electrolyte		. .	(6) $H_2O_{(l)}$.	(6) $H^+, H_2O_{(l)}$[a] $\mathit{O^{2-}}$	. .
Cathode	Catalyst	(1) $N_2, O_2, H_2O_{(g)}, H_2O_{(l)}$ (1) $\mathit{N_2, O_2}$	(5) $N_2, O_2, H_2O_{(g)}, H_2O_{(l)}$ (5) $\mathit{N_2, O_2}$	(3)(5) e^-, H^+ (3)(5) $\mathit{e^-, O^{2-}}$	(6) $2H^+ + \frac{1}{2}O_2 + 2e^- \rightarrow H_2O_{(l)}$ $\mathit{\frac{1}{2}O_2 + 2e^- \rightarrow O^{2-}}$
	Electrode	(1) $N_2, O_2, H_2O_{(g)}, H_2O_{(l)}$ (1) $\mathit{N_2, O_2}$	(6) $N_2, O_2, H_2O_{(g)}, H_2O_{(l)}$ $\mathit{N_2, O_2}$	(3) e^- (3)(5) $\mathit{e^-, O^{2-}}$	. (5) $\mathit{\frac{1}{2}O_2 + 2e^- \rightarrow O^{2-}}$
	Flow Channels	(1) $N_2, O_2, H_2O_{(g)}$ (1) $\mathit{N_2, O_2}$	(2) $N_2, O_2, H_2O_{(g)}, H_2O_{(l)}$ (2) $\mathit{N_2, O_2}$	(3) e^- (3) $\mathit{e^-}$	. .

Table 6.2: Description of a full PEMFC (or SOFC in italics) model. Six key assumptions, numbered (1-6) in parentheses, lead to the simplified model shown in table 6.3.

[a] To be precise, this water transport phenomenon is due to electro-osmotic drag (See chapter 4). For convenience, it has been categorized as conduction due to its close relationship with proton conduction.

2. Ignore diffusion in in flow channels

Simplifying Model

Domains \ Phenomena		Convection	Diffusion	Conduction	Electrochemical Reaction
Anode	Flow Channels	(1) $H_2, H_2O_{(g)}, H_2O_{(l)}$ (1) *$H_2, H_2O_{(g)}$*	(2) $H_2, H_2O_{(g)}, H_2O_{(l)}$ (2) *$H_2, H_2O_{(g)}$*	(3) e^- (3) *e^-*	. .
	Electrode	(1) $H_2, H_2O_{(g)}, H_2O_{(l)}$ (1) *$H_2, H_2O_{(g)}$*	(6) $H_2, H_2O_{(g)}, H_2O_{(l)}$ *$H_2, H_2O_{(g)}$*	(3) e^- (3)(5) *e^-, O^{2-}*	. (5) *$H_2 + O^{2-} \rightarrow H_2O + 2e^-$*
	Catalyst	(1) $H_2, H_2O_{(g)}, H_2O_{(l)}$ (1) *$H_2, H_2O_{(g)}$*	(5) $H_2, H_2O_{(g)}, H_2O_{(l)}$ (5) *$H_2, H_2O_{(g)}$*	(3)(5) e^-, H^+ (3)(5) *e^-, O^{2-}*	(4) $H_2 \rightarrow 2H^+ + 2e^-$ *$H_2 + O^{2-} \rightarrow H_2O + 2e^-$*
Electrolyte		. .	(6) $H_2O_{(l)}$.	(6) $H^+, H_2O_{(l)}$[a] *O^{2-}*	. .
Cathode	Catalyst	(1) $N_2, O_2, H_2O_{(g)}, H_2O_{(l)}$ (1) *N_2, O_2*	(5) $N_2, O_2, H_2O_{(g)}, H_2O_{(l)}$ (5) *N_2, O_2*	(3)(5) e^-, H^+ (3)(5) *e^-, O^{2-}*	(6) $2H^+ + \frac{1}{2}O_2 + 2e^- \rightarrow H_2O_{(l)}$ *$\frac{1}{2}O_2 + 2e^- \rightarrow O^{2-}$*
	Electrode	(1) $N_2, O_2, H_2O_{(g)}, H_2O_{(l)}$ (1) *N_2, O_2*	(6) $N_2, O_2, H_2O_{(g)}, H_2O_{(l)}$ *N_2, O_2*	(3) e^- (3)(5) *e^-, O^{2-}*	. (5) *$\frac{1}{2}O_2 + 2e^- \rightarrow O^{2-}$*
	Flow Channels	(1) $N_2, O_2, H_2O_{(g)}$ (1) *N_2, O_2*	(2) $N_2, O_2, H_2O_{(g)}, H_2O_{(l)}$ (2) *N_2, O_2*	(3) e^- (3) *e^-*	. .

Table 6.2: Description of a full PEMFC (or SOFC in italics) model. Six key assumptions, numbered (1-6) in parentheses, lead to the simplified model shown in table 6.3.

[a] To be precise, this water transport phenomenon is due to electro-osmotic drag (See chapter 4). For convenience, it has been categorized as conduction due to its close relationship with proton conduction.

3. Ignore electronic resistances

Simplifying Model

Domains \ Phenomena		Convection	Diffusion	Conduction	Electrochemical Reaction
Anode	Flow Channels	(1) $H_2, H_2O_{(g)}, H_2O_{(l)}$ (1) *$H_2, H_2O_{(g)}$*	(2) $H_2, H_2O_{(g)}, H_2O_{(l)}$ (2) *$H_2, H_2O_{(g)}$*	(3) e^- (3) *e^-*	. .
	Electrode	(1) $H_2, H_2O_{(g)}, H_2O_{(l)}$ (1) *$H_2, H_2O_{(g)}$*	(6) $H_2, H_2O_{(g)}, H_2O_{(l)}$ *$H_2, H_2O_{(g)}$*	(3) e^- (3)(5) *e^-, O^{2-}*	. (5) *$H_2 + O^{2-} \rightarrow H_2O + 2e^-$*
	Catalyst	(1) $H_2, H_2O_{(g)}, H_2O_{(l)}$ (1) *$H_2, H_2O_{(g)}$*	(5) $H_2, H_2O_{(g)}, H_2O_{(l)}$ (5) *$H_2, H_2O_{(g)}$*	(3)(5) e^-, H^+ (3)(5) *e^-, O^{2-}*	(4) $H_2 \rightarrow 2H^+ + 2e^-$ *$H_2 + O^{2-} \rightarrow H_2O + 2e^-$*
Electrolyte		. .	(6) $H_2O_{(l)}$.	(6) $H^+, H_2O_{(l)}$ [a] *O^{2-}*	. .
Cathode	Catalyst	(1) $N_2, O_2, H_2O_{(g)}, H_2O_{(l)}$ (1) *N_2, O_2*	(5) $N_2, O_2, H_2O_{(g)}, H_2O_{(l)}$ (5) *N_2, O_2*	(3)(5) e^-, H^+ (3)(5) *e^-, O^{2-}*	(6) $2H^+ + \frac{1}{2}O_2 + 2e^- \rightarrow H_2O_{(l)}$ *$\frac{1}{2}O_2 + 2e^- \rightarrow O^{2-}$*
	Electrode	(1) $N_2, O_2, H_2O_{(g)}, H_2O_{(l)}$ (1) *N_2, O_2*	(6) $N_2, O_2, H_2O_{(g)}, H_2O_{(l)}$ *N_2, O_2*	(3) e^- (3)(5) *e^-, O^{2-}*	. (5) *$\frac{1}{2}O_2 + 2e^- \rightarrow O^{2-}$*
	Flow Channels	(1) $N_2, O_2, H_2O_{(g)}$ (1) *N_2, O_2*	(2) $N_2, O_2, H_2O_{(g)}, H_2O_{(l)}$ (2) *N_2, O_2*	(3) e^- (3) *e^-*	. .

Table 6.2: Description of a full PEMFC (or SOFC in italics) model. Six key assumptions, numbered (1-6) in parentheses, lead to the simplified model shown in table 6.3.

[a] To be precise, this water transport phenomenon is due to electro-osmotic drag (See chapter 4). For convenience, it has been categorized as conduction due to its close relationship with proton conduction.

4. Ignore anodic reaction loss

Simplifying Model

Domains \ Phenomena		Convection	Diffusion	Conduction	Electrochemical Reaction
Anode	Flow Channels	(1) $H_2, H_2O_{(g)}, H_2O_{(l)}$ (1) *$H_2, H_2O_{(g)}$*	(2) $H_2, H_2O_{(g)}, H_2O_{(l)}$ (2) *$H_2, H_2O_{(g)}$*	(3) e^- (3) *e^-*	. .
	Electrode	(1) $H_2, H_2O_{(g)}, H_2O_{(l)}$ (1) *$H_2, H_2O_{(g)}$*	(6) $H_2, H_2O_{(g)}, H_2O_{(l)}$ *$H_2, H_2O_{(g)}$*	(3) e^- (3)(5) *e^-, O^{2-}*	. (5) *$H_2 + O^{2-} \rightarrow H_2O + 2e^-$*
	Catalyst	(1) $H_2, H_2O_{(g)}, H_2O_{(l)}$ (1) *$H_2, H_2O_{(g)}$*	(5) $H_2, H_2O_{(g)}, H_2O_{(l)}$ (5) *$H_2, H_2O_{(g)}$*	(3)(5) e^-, H^+ (3)(5) *e^-, O^{2-}*	(4) $H_2 \rightarrow 2H^+ + 2e^-$ *$H_2 + O^{2-} \rightarrow H_2O + 2e^-$*
Electrolyte		. .	(6) $H_2O_{(l)}$.	(6) $H^+, H_2O_{(l)}$[a] *O^{2-}*	. .
Cathode	Catalyst	(1) $N_2, O_2, H_2O_{(g)}, H_2O_{(l)}$ (1) *N_2, O_2*	(5) $N_2, O_2, H_2O_{(g)}, H_2O_{(l)}$ (5) *N_2, O_2*	(3)(5) e^-, H^+ (3)(5) *e^-, O^{2-}*	(6) $2H^+ + \frac{1}{2}O_2 + 2e^- \rightarrow H_2O_{(l)}$ *$\frac{1}{2}O_2 + 2e^- \rightarrow O^{2-}$*
	Electrode	(1) $N_2, O_2, H_2O_{(g)}, H_2O_{(l)}$ (1) *N_2, O_2*	(6) $N_2, O_2, H_2O_{(g)}, H_2O_{(l)}$ *N_2, O_2*	(3) e^- (3)(5) *e^-, O^{2-}*	. (5) *$\frac{1}{2}O_2 + 2e^- \rightarrow O^{2-}$*
	Flow Channels	(1) $N_2, O_2, H_2O_{(g)}$ (1) *N_2, O_2*	(2) $N_2, O_2, H_2O_{(g)}, H_2O_{(l)}$ (2) *N_2, O_2*	(3) e^- (3) *e^-*	. .

Table 6.2: Description of a full PEMFC (or SOFC in italics) model. Six key assumptions, numbered (1-6) in parentheses, lead to the simplified model shown in table 6.3.

[a] To be precise, this water transport phenomenon is due to electro-osmotic drag (See chapter 4). For convenience, it has been categorized as conduction due to its close relationship with proton conduction.

5. Thin catalyst layer (Ignore transport loss)

Simplifying Model

Domains \ Phenomena		Convection	Diffusion	Conduction	Electrochemical Reaction
Anode	Flow Channels	(1) $H_2, H_2O_{(g)}, H_2O_{(l)}$ (1) $H_2, H_2O_{(g)}$	(2) $H_2, H_2O_{(g)}, H_2O_{(l)}$ (2) $H_2, H_2O_{(g)}$	(3) e^- (3) e^-	. .
	Electrode	(1) $H_2, H_2O_{(g)}, H_2O_{(l)}$ (1) $H_2, H_2O_{(g)}$	(6) $H_2, H_2O_{(g)}, H_2O_{(l)}$ $H_2, H_2O_{(g)}$	(3) e^- (3)(5) e^-, O^{2-}	. (5) $H_2 + O^{2-} \rightarrow H_2O + 2e^-$
	Catalyst	(1) $H_2, H_2O_{(g)}, H_2O_{(l)}$ (1) $H_2, H_2O_{(g)}$	(5) $H_2, H_2O_{(g)}, H_2O_{(l)}$ (5) $H_2, H_2O_{(g)}$	(3)(5) e^-, H^+ (3)(5) e^-, O^{2-}	(4) $H_2 \rightarrow 2H^+ + 2e^-$ $H_2 + O^{2-} \rightarrow H_2O + 2e^-$
Electrolyte		. .	(6) $H_2O_{(l)}$.	(6) $H^+, H_2O_{(l)}$[a] O^{2-}	. .
Cathode	Catalyst	(1) $N_2, O_2, H_2O_{(g)}, H_2O_{(l)}$ (1) N_2, O_2	(5) $N_2, O_2, H_2O_{(g)}, H_2O_{(l)}$ (5) N_2, O_2	(3)(5) e^-, H^+ (3)(5) e^-, O^{2-}	(6) $2H^+ + \frac{1}{2}O_2 + 2e^- \rightarrow H_2O_{(l)}$ $\frac{1}{2}O_2 + 2e^- \rightarrow O^{2-}$
	Electrode	(1) $N_2, O_2, H_2O_{(g)}, H_2O_{(l)}$ (1) N_2, O_2	(6) $N_2, O_2, H_2O_{(g)}, H_2O_{(l)}$ N_2, O_2	(3) e^- (3)(5) e^-, O^{2-}	. (5) $\frac{1}{2}O_2 + 2e^- \rightarrow O^{2-}$
	Flow Channels	(1) $N_2, O_2, H_2O_{(g)}$ (1) N_2, O_2	(2) $N_2, O_2, H_2O_{(g)}, H_2O_{(l)}$ (2) N_2, O_2	(3) e^- (3) e^-	. .

Table 6.2: Description of a full PEMFC (or SOFC in italics) model. Six key assumptions, numbered (1-6) in parentheses, lead to the simplified model shown in table 6.3.

[a] To be precise, this water transport phenomenon is due to electro-osmotic drag (See chapter 4). For convenience, it has been categorized as conduction due to its close relationship with proton conduction.

6. Single phase assumption (no liquid water)

Simplified Model

Domains \ Reactions		Convection	Diffusion	Conduction	Electrochemical Reaction
Anode	Flow Channels	.	.	.	.
	Electrode	. .	H_2, $H_2O_{(g)}$ $\mathit{H_2}$, $\mathit{H_2O_{(g)}}$	. .	. .
	Catalyst	. .	. .	. .	. $\mathit{H_2+O^{2-} \rightarrow H_2O_{(g)}+2e^-}$
Electrolyte		. .	$H_2O_{(g)}$.	H^+, $H_2O_{(g)}$ $\mathit{O^{2-}}$	. .
Cathode	Catalyst	. .	. .	. .	$2H^+ + \frac{1}{2}O_2 + 2e^- \rightarrow H_2O_{(g)}$ $\mathit{\frac{1}{2}O_2+2e^- \rightarrow O^{2-}}$
	Electrode	. .	N_2, O_2, $H_2O_{(g)}$ $\mathit{N_2}$, $\mathit{O_2}$	. .	. .
	Flow Channels	.	.	.	.

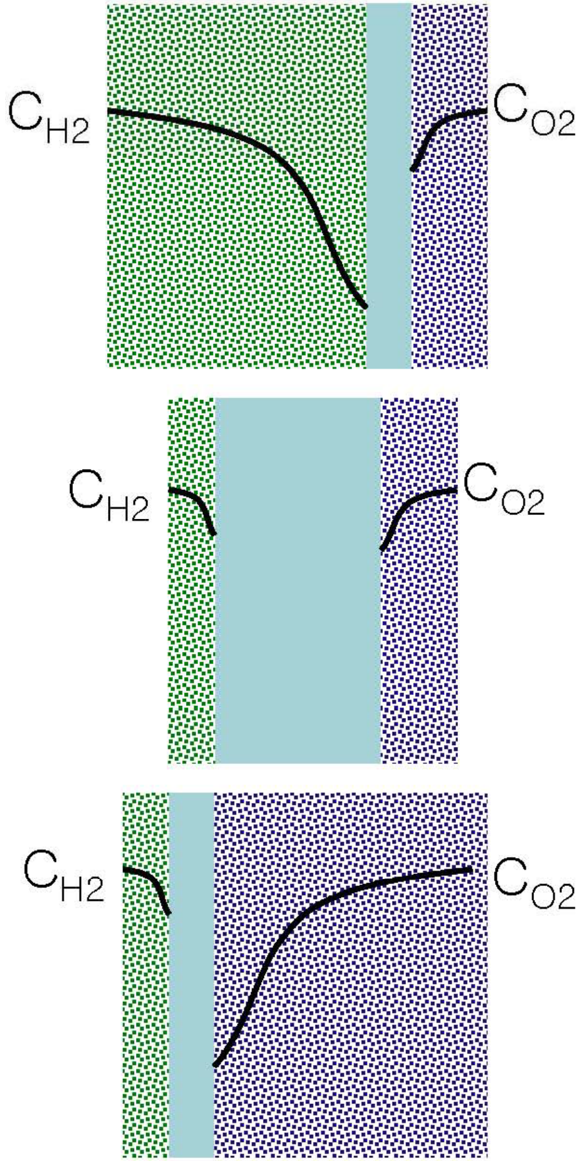
Table 6.3: Description of a simplified PEMFC (or SOFC in italics) model. The items to be modeled in this table are described by governing equations which are developed in next section.

Model Validity For SOFCs

Anode supported

Electrolyte supported

Cathode supported



Governing Equations: Electrode

Diffusion model

Binary diffusion $J_i = -D_{ij}\frac{dc_i}{dx}$ $J_j = -D_{ji}\frac{dc_j}{dz}$ $D_{ij} = D_{ji}.$

Maxwell-Stefan $$\frac{dx_i}{dz} = RT\sum_{j\neq i}\frac{x_iJ_j - x_jJ_i}{PD_{ij}^{eff}}$$

For simplicity, we use

$$J_i = \frac{-pD_{ij}^{eff}}{RT}\frac{dx_i}{dz}$$

Governing Equations: Electrolyte

SOFC

$$\eta_{ohmic} = j(ASR_{ohmic}) = j(\frac{t^M}{\sigma})$$

$$\sigma = \frac{Ae^{\frac{\Delta G_{act}}{RT}}}{T}$$

PEMFC

$$J^M_{H_2O} = 2n_{drag}\frac{j}{2F}\frac{\lambda}{22} - \frac{\rho_{dry}}{M_m}D_\lambda\frac{d\lambda}{dz}$$

Governing Equations: Catalyst

Simplified B-V

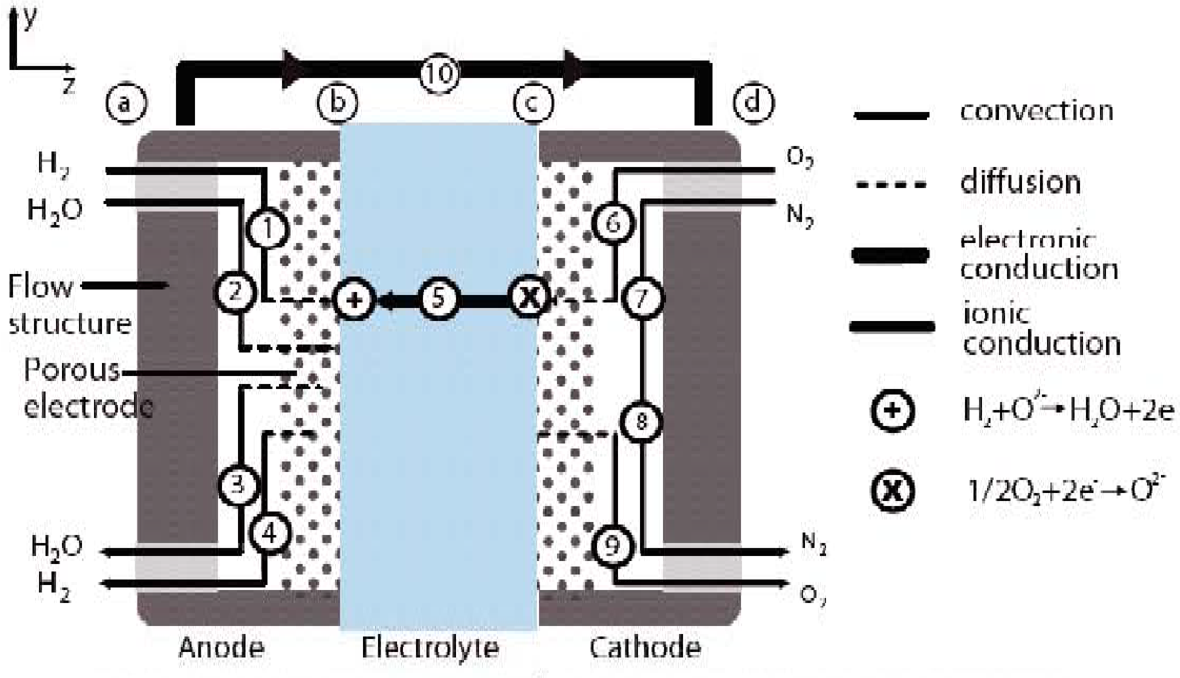
$$j = j_0^0 \left(\frac{c_R^*}{c_R^{0*}} e^{\left(\frac{\alpha n F \eta_{act}}{RT} \right)} \right)$$

$$\eta_{cathode} = \frac{RT}{4\alpha F} \ln \frac{j c_{O_2}^0}{j_0 c_{O_2}}$$

For ideal gas

$$\eta_{cathode} = \frac{RT}{4\alpha F} \ln \frac{j}{j_0} p^C x_{O_2}$$

Example 1: 1-D SOFC



(b) In a SOFC, oxygen ions(O^{2-}) transport through the electrolyte.

Anode

$$J^A_{H_2} = \frac{-p^A D^{eff}_{H_2,H_2O}}{RT}\frac{dx_{H_2}}{dz}$$

$$J^A_{H_2O} = \frac{-p^A D^{eff}_{H_2,H_2O}}{RT}\frac{dx_{H_2O}}{dz}$$

$$x_{H_2}|_b = x_{H_2}|_a - t^A \frac{jRT}{2Fp^A D^{eff}_{H_2,H_2O}}$$

$$x_{H_2O}|_b = x_{H_2O}|_a + t^A \frac{jRT}{2Fp^A D^{eff}_{H_2,H_2O}}$$

Cathode

$$x_{O_2}|_c - x_{O_2}|_d - t^C \frac{jRT}{4Fp^C D^{eff}_{O_2,N_2}}$$

Example 1: 1-D SOFC

Cathodic overvotalge

$$\eta_{ohmic} = jR = j\frac{t^M}{sigma} = j\frac{t^M T}{Ae^{\frac{\Delta G_{act}}{RT}}}$$

Ohmic overvoltage

$$\eta_{cathode} = \frac{RT}{4\alpha F}\ln\left[\frac{j}{j_0 p^C\left(x_{O_2}|_d - t^C\frac{jRT}{4Fp^C D^{eff}_{O_2,N_2}}\right)}\right]$$

Overall

$$V = E_{thermo} - \eta_{ohmic} - \eta_{cathode} \quad (6$$

$$= E_{thermo} - j\frac{t^M T}{Ae^{\frac{\Delta G_{act}}{RT}}} - \frac{RT}{4\alpha F}\ln\left[\frac{j}{j_0 p^C\left(x_{O_2}|_d - t^C\frac{jRT}{4Fp^C D^{eff}_{O_2,N_2}}\right)}\right]$$

Example 1: 1-D SOFC

For j=500mA/cm^2

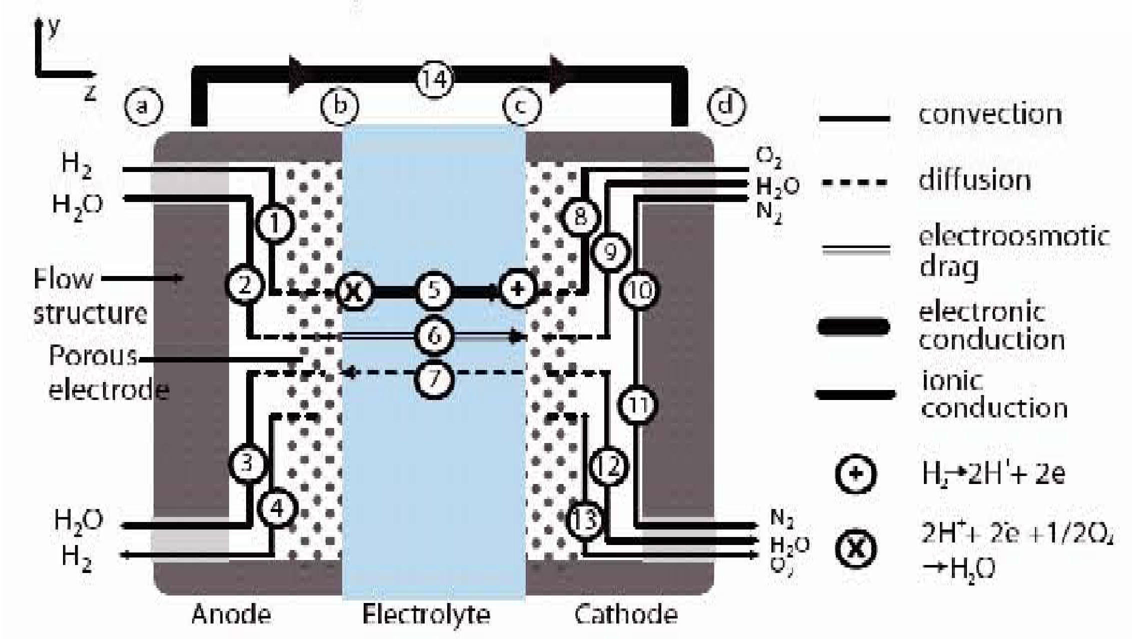
Physical properties	Values
Thermodynamic voltage, E_{thermo} (V)	1.0
Temperature, T(K)	1073
Hydrogen inlet mole fraction, $x_{H_2}\|_a$	0.95
Oxygen inlet mole fraction, $x_{O_2}\|_d$	0.21
Cathode pressure, p^C(atm)	1
Anode pressure, p^A(atm)	1
Effective Hydrogen (or water) diffusivity, $D^{eff}_{H_2,H_2O}(m^2/s)$	1×10^{-4}
Effective Oxygen diffusivity, $D^{eff}_{O_2,N_2}(m^2/s)$	2×10^{-5}
Transfer coefficient, α	0.5
Exchange current density, $j_0(A/cm^2)$	0.1
Electrolyte constant, Λ(K/Ωm)	0.001
Electrolyte Activation energy, ΔG_{act}(kJ/mol)	100
Electrolyte thickness, t^M (μm)	10
Anode thickness, t^A(μm)	50
Cathode thickness t^C(μm)	800
Gas constant, R(J/mol K)	8.314
Faraday constant, F(C/mol)	96485

$$\eta_{ohmic} = 0.1A/cm^2 \frac{0.00001m \cdot 1073K}{0.001S \cdot K/m \; e^{\frac{100000kJ/mol}{8.314J/mol\cdot K \;\; 1073K}}}$$
$$= 0.1A/cm^2 \times 1.45 \cdot 10^{-4}\Omega m^2 = 0.145V$$

$$\eta_{cathodic} - \frac{8.314\frac{J}{mol\;K}1073K}{4\cdot 0.5\cdot 96485\frac{C}{mol}} \ln\left[\frac{0.5\frac{A}{cm^2}}{0.1\frac{A}{cm^2}\cdot 1atm} \times \frac{1}{\left(0.21 - 0.0008m\frac{0.5\frac{A}{cm^2}8.314\frac{J}{mol\;K}1073K}{4\cdot 96485\frac{C}{mol}101325Pa\cdot 0.00002\frac{m^2}{s}}\right)}\right]$$
$$= 0.147V$$

$$V = 1.0V - 0.145V - 0.147V = 0.708V$$

Example 2: 1-D PEMFC



(a) In a PEMFC, water(H_2O) and proton(H^+) transport through the electrolyte.

Anode

$$J^A_{H_2} = \frac{-p^A D^{eff}_{H_2,H_2O}}{RT}\frac{dx_{H_2}}{dz} \qquad x_{H_2}|_b = x_{H_2}|_a - t^A \frac{jRT}{2Fp^A D^{eff}_{H_2,H_2O}}$$

$$J^A_{H_2O} = \frac{-p^A D^{eff}_{H_2,H_2O}}{RT}\frac{dx_{H_2O}}{dz} \qquad x_{H_2O}|_b = x_{H_2O}|_a - t^A \frac{\alpha^* jRT}{2Fp^A D^{eff}_{H_2,H_2O}}$$

Cathode

$$x_{O_2}|_c = x_{O_2}|_d - t^C \frac{jRT}{4Fp^C D^{eff}_{O_2,H_2O}}$$

$$x_{H_2O}|_c = x_{H_2O}|_d + t^C \frac{(1+\alpha^*)jRT}{2Fp^C D^{eff}_{O_2,H_2O}}$$

Example 2: 1-D PEMFC

Nafion model from Chapter 4 with constant water diffusivity

$$\lambda(z) = \frac{11\alpha^*}{n_{drag}^{SAT}} + C\exp\left[\frac{jM_m n_{drag}^{SAT}}{22F\rho_{dry}D_\lambda}z\right] = \frac{11\alpha^*}{2.5}$$

$$+C\exp\left[\frac{j[A/cm^2] \times 1.0kg/mol \times 2.5}{22 \times 96500C/mol \times 0.00197kg/cm^3 \times D_\lambda[cm^2/s]}z\right]$$

$$= 4.4\alpha^* + C\exp\left(\frac{0.000598 \cdot j[A/cm^2] \cdot z[cm]}{D_\lambda[cm^2/s]}\right) \quad (6$$

$$\lambda|_b = \lambda(0) = 4.4\alpha^* + C$$

$$\lambda|_c = \lambda(t^M) = 4.4\alpha^* + C\exp\left(\frac{0.000598 \cdot j[A/cm^2] \cdot t^M[cm]}{D_\lambda[cm^2/s]}\right)$$

Example 2: 1-D PEMFC

Linearized water contents at Nafion surface

$$\lambda = 14a_W \quad \text{for} \quad 0 < a_W \leq 1$$
$$\lambda = 12.6 + 1.4a_W \quad \text{for} \quad 1 < a_W \leq 3$$

using $a_W|_b = \frac{p^C x_{H_2O}|_b}{p_{SAT}}$,

$$\lambda|_b = 14a_W|_b = 14\frac{p^C}{p_{SAT}}\left(x_{H_2O}|_a - t^A \frac{\alpha^* jRT}{2Fp^A D^{eff}_{H_2,H_2O}}\right)$$

$$\lambda|_c = 12.6 + 1.4a_W|_c = 12.6 + 1.4\frac{p^C}{p_{SAT}}\left(x_{H_2O}|_d + t^C \frac{(1+\alpha^*)jRT}{2Fp^C D^{eff}_{O_2,H_2O}}\right)$$

Example 2: 1-D PEMFC

Physical properties	Values
Thermodynamic voltage, E_{thermo}(V)	1.0
Operating current density, j(A/cm^2)	0.5
Temperature, T(K)	343
Vapor saturation pressure, p_{SAT}(atm)	0.307
Hydrogen mole fraction, x_{H_2}	0.9
Oxygen mole fraction, x_{O_2}	0.19
Cathode water mole fraction, x_{H_2O}	0.1
Cathode pressure, p^C(atm)	3
Anode pressure, p^A(atm)	3
Effective hydrogen (or water) diffusivity, $D^{eff}_{H_2,H_2O}(cm^2/s)$	0.149
Effective oxygen (or water) diffusivity, $D^{eff}_{O_2,H_2O}(cm^2/s)$	0.0295
Water diffusivity in Nafion®, $D_\lambda(cm^2/s)$	3.81×10^{-6}
Transfer coefficient, α	0.5
Exchange current density, $j_0(A/cm^2)$	0.0001
Electrolyte thickness, t^M(μm)	125
Anode thickness, t^A(μm)	350
Cathode thickness t^C(μm)	350
Gas constant, R(J/mol K)	8.314
Faraday constant, F(C/mol)	96485

Example 2: 1-D PEMFC

$$\lambda|_b = 14\frac{3atm}{0.307atm}\left(0.1 - 0.00035m\frac{\alpha^* \cdot 0.5\frac{A}{0.0001m^2} \cdot 8.314\frac{J}{molK} \cdot 343K}{2 \cdot 96485\frac{C}{mol} \cdot 3 \times 101325Pa \cdot 0.149\frac{0.0001m^2}{s}}\right)$$

$$= 13.68 - 0.781\alpha^* \qquad (6.47)$$

$$\lambda|_c = 12.6 + 1.4\frac{3atm}{0.307atm}\left(0.1 + 0.00035m\frac{(1+\alpha^*)0.5\frac{A}{0.0001m^2} \cdot 8.314\frac{J}{molK} \cdot 343K}{2 \cdot 96485\frac{C}{mol} \cdot 3 \times 101325Pa \cdot 0.0295\frac{0.0001m^2}{s}}\right)$$

$$= 14.36 + 0.394\alpha^* \qquad (6.48)$$

$$\lambda|_b = \lambda(0) = 4.4\alpha^* + C$$

$$\lambda|_c = 4.4\alpha^* + C\exp\left(\frac{0.000598 \cdot 0.5A/cm^2 \cdot 0.0125cm}{3.81 \times 10^{-6}}\right)$$

$$= 4.4\alpha^* + 2.667C$$

$\alpha = 2.25$ and $C = 2.0.$

Example 2: 1-D PEMFC

$$\sigma(z) = \left[0.005193(4.4\alpha + C\exp(\frac{0.000598 \cdot 0.5 \cdot}{3.81 \times 10^{-6}} z)) - 0.00326\right]$$
$$\times \exp\left[1268\left(\frac{1}{303} - \frac{1}{343}\right)\right]$$
$$= 0.0784 + 0.0169\exp(78.48z)$$

$$R_m = \int_0^{t_m} \frac{dz}{\sigma(z)} = \int_0^{0.0125} \frac{dz}{0.0784 + 0.0169\exp(78.48z)}$$
$$= 0.117\Omega cm^2$$

$$\eta_{ohmic} = j \times R_m = 0.5(A/cm^2) \times 0.117(\Omega cm^2) = 0.0585V$$

Example 2: 1-D PEMFC

$$\eta_{cathode} = \frac{RT}{4\alpha F} \ln \left[\frac{j}{j_0 p^C \left(x_{O_2}|_d - t^C \frac{jRT}{4Fp^C D^{eff}_{O_2,N_2}} \right)} \right]$$

$$\eta_{cathodic} = \frac{8.314 \frac{J}{mol\ K} 343K}{4 \cdot 0.5 \cdot 96485 \frac{C}{mol}} \ln \left[\frac{0.5 \frac{A}{cm^2}}{0.0001 \frac{A}{cm^2} \cdot 3atm} \times \right.$$

$$\left. \frac{1}{\left(0.19 - 0.00035m \frac{0.5 \frac{A}{cm^2} 8.314 \frac{J}{mol\ K} 343K}{4 \cdot 96485 \frac{C}{mol} 3 \cdot 101325 Pa \cdot 0.0295 \times 10^{-4} \frac{m^2}{s}} \right)} \right]$$

$$= 0.134V$$

$$V = 1.0V - 0.0585V - 0.134V = 0.807V$$

Example 3: 1-D SOFC

Stoichiometric number

$$\lambda_{H_2} = \frac{J_{H_2,inlet}}{J^A_{H_2}}$$

$$\lambda_{O_2} = \frac{J_{O_2,inlet}}{J^C_{O_2}}$$

$$x_{O_2}|_d = \frac{J^C_{O_2,outlet}}{J^C_{O_2,outlet} + J^C_{N_2,outlet}}$$

$$J^C_{O_2,outlet} = J^C_{O_2,inlet} - J^C_{O_2} = J^C_{O_2,inlet} - \frac{j}{4F}$$

$$J^C_{O_2,inlet} = \lambda_{O_2} J^C_{O_2}$$

$$J^C_{O_2,outlet} = (\lambda_{O_2} - 1) J^C_{O_2} = (\lambda_{O_2} - 1)\frac{j}{4F}$$

$$J^C_{N_2,outlet} = J^C_{N_2,inlet} = \omega J^C_{O_2,inlet} = \omega\lambda_{O_2} J^C_{O_2} = \omega\lambda_{O_2}\frac{j}{4F}$$

$$\omega = 0.79/0.21 = 3.76$$

$$x_{O_2}|_d = \frac{(\lambda_{O_2} - 1)\frac{j}{4F}}{(\lambda_{O_2} - 1)\frac{j}{4F} + \omega\lambda_{O_2}\frac{j}{4F}} = \frac{\lambda_{O_2} - 1}{(1+\omega)\lambda_{O_2} - 1}$$

Example 3: 1-D SOFC

$$\eta_{cathode} = \frac{RT}{4\alpha F} \ln \left[\frac{j}{j_0 p^C \left(x_{O_2}|_d - t^C \frac{jRT}{4Fp^C D^{eff}_{O_2,N_2}} \right)} \right]$$

$$\begin{aligned} V &= E_{thermo} - \eta_{ohmic} - \eta_{cathode} \\ &= E_{thermo} - j \frac{t^M T}{A e^{\frac{\Delta G_{act}}{RT}}} \\ &\quad - \frac{RT}{4\alpha F} \ln \left[\frac{j}{j_0 p^C \left(\frac{\lambda_{O_2} - 1}{(1+\omega)\lambda_{O_2} - 1} - t^C \frac{jRT}{4Fp^C D^{eff}_{O_2,N_2}} \right)} \right] \end{aligned}$$

Example 3: 1-D SOFC

$\lambda_{O_2} = 1.2$ and j=$500 mA/cm^2$

$$\eta_{cathodic} = \frac{8.314 \frac{J}{mol\ K} 1073K}{4 \cdot 0.5 \cdot 96485 \frac{C}{mol}} \ln \left[\frac{0.5 \frac{A}{cm^2}}{0.1 \frac{A}{cm^2} \cdot 1atm} \times \right.$$

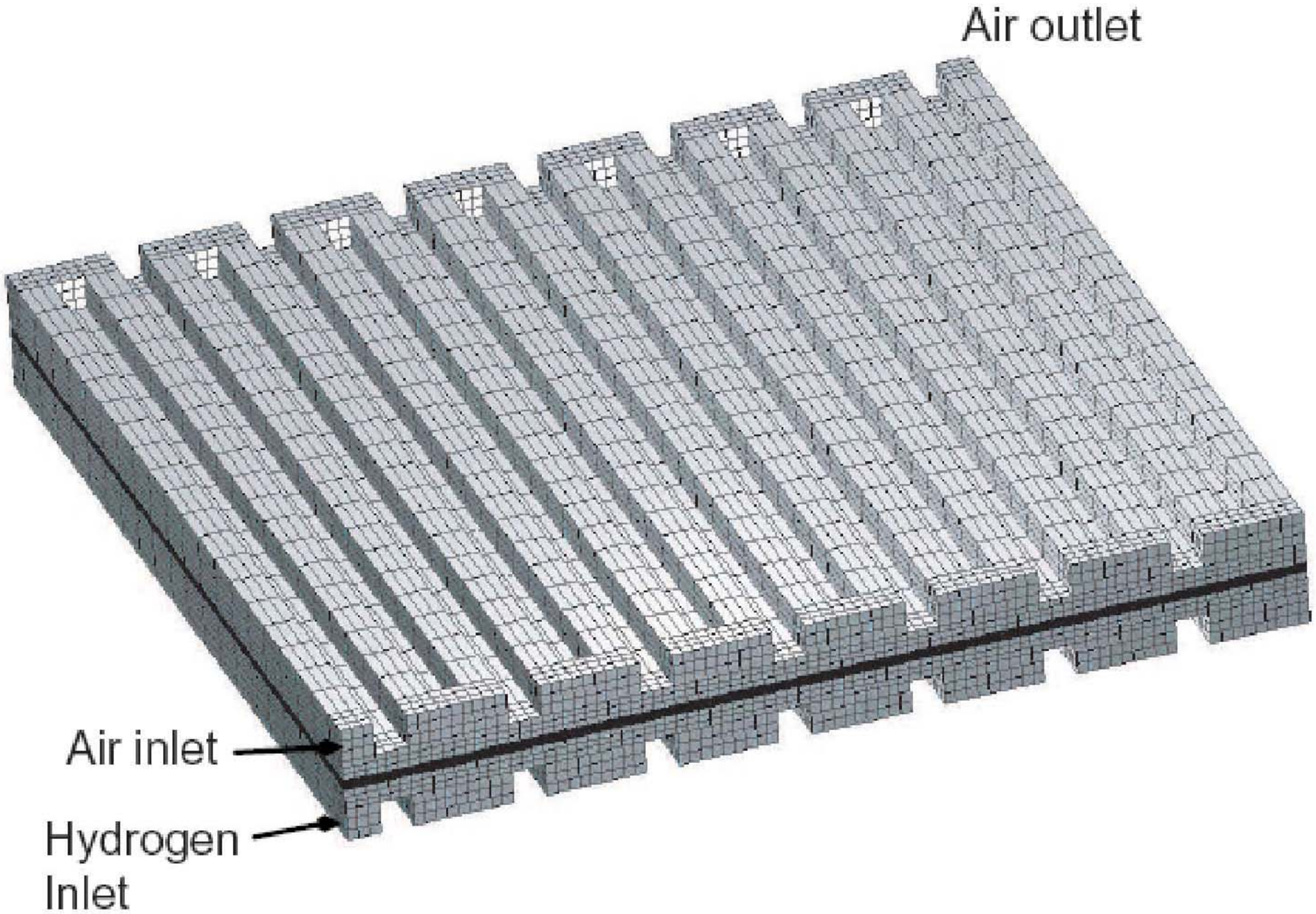
$$\left. \frac{1}{\left(\frac{1.2-1}{(1+3.76)1.2-1} - 0.0008m \frac{0.5 \frac{A}{cm^2} 8.314 \frac{J}{mol\ K} 1073K}{4 \cdot 96485 \frac{C}{mol} 101325Pa \cdot 0.00002 \frac{m^2}{s}} \right)} \right]$$

$$= 0.219V$$

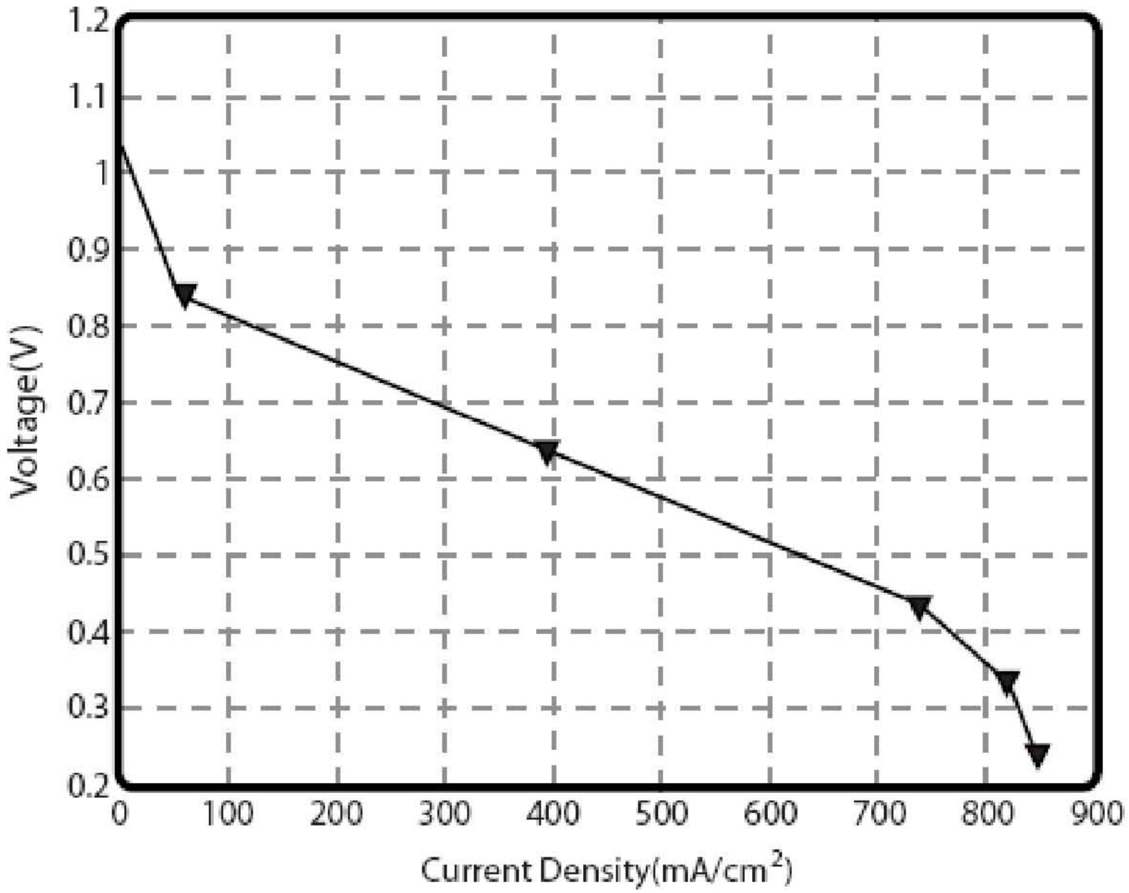
$$V = 1.0V - 0.145V - 0.219V = 0.636V$$

Compare with cathodic overpotential of 0.147V in example 1

Computational Fuel Cell Dynamics(CFCD)



Computational Fuel Cell Dynamics(CFCD)



Computational Fuel Cell Dynamics(CFCD)

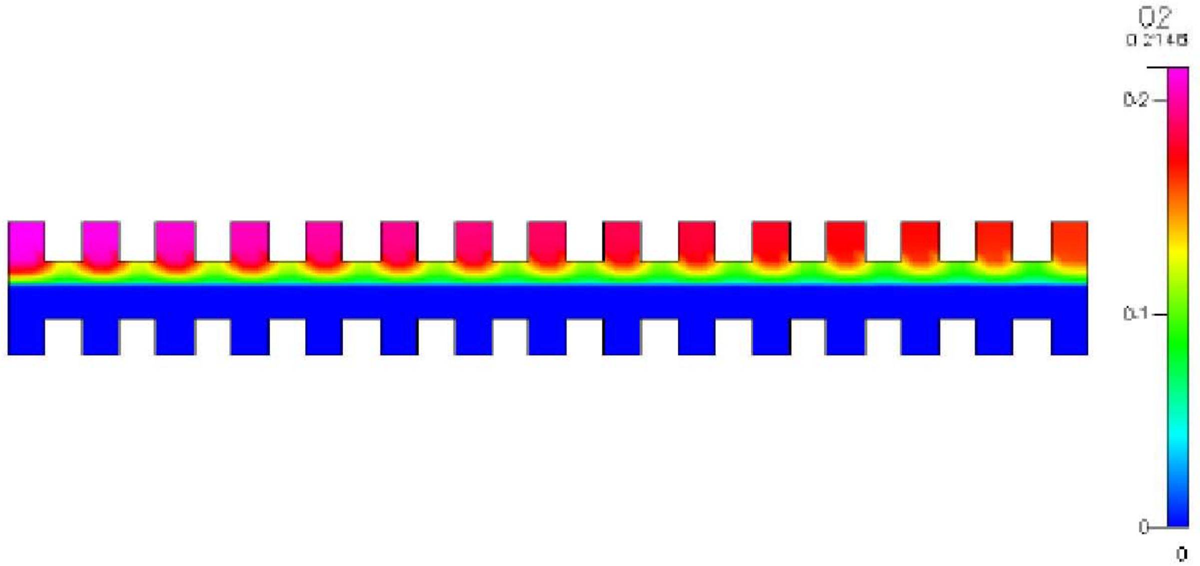


Figure 6.7: Oxygen concentration in the cathode at 0.8V overvoltage. This cross-sectional cut across the center of the serpentine pattern illustrates how the oxygen concentration in the flow channel slowly decreases from inlet to outlet.

Computational Fuel Cell Dynamics(CFCD)

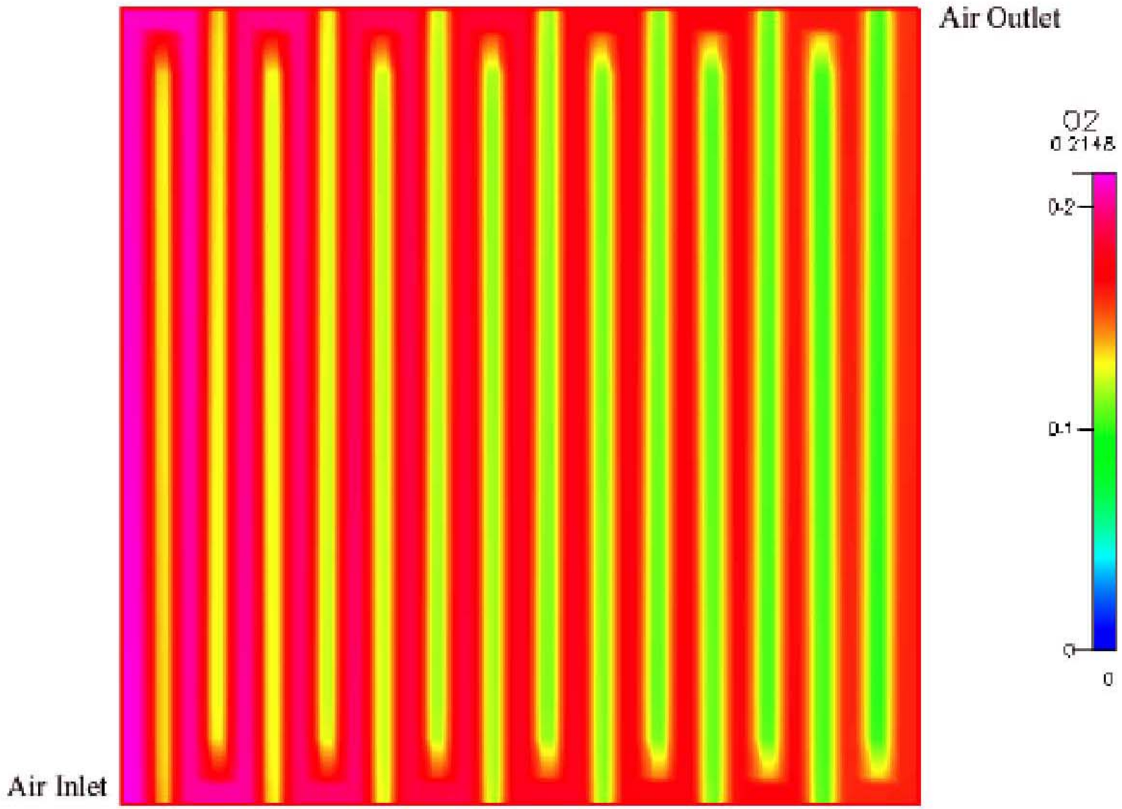


Figure 6.8: Oxygen concentration in the cathode at 0.8 V overvoltage. The plan-view figure shows the oxygen concentration profile across the cathode surface. Low oxygen concentration is observed under the channel ribs due to the blockage of oxygen flux.

Computational Fuel Cell Dynamics(CFCD)

Category	Equations
1. Mass conservation	$\frac{\partial}{\partial t}(\epsilon\rho) + \nabla \cdot (\epsilon\rho\mathbf{U}) = 0$
2. Momentum conservation	$\frac{\partial}{\partial t}(\epsilon\rho\mathbf{U}) + \nabla \cdot (\epsilon\rho\mathbf{U}\mathbf{U}) = -\epsilon\nabla p + \nabla \cdot (\epsilon\zeta) + \frac{\epsilon^2\mu\mathbf{U}}{\kappa}$
3. Species conservation	$\frac{\partial}{\partial t}(\epsilon\rho X_i) + \nabla \cdot (\epsilon\rho\mathbf{U}X_i) = \nabla \cdot \mathbf{J}_i + S_i$
4. Charge conservation	$\nabla \cdot \mathbf{i}_{elec} = -\nabla \cdot \mathbf{i}_{ion}$

1. Mass conservation

$$\underbrace{\frac{\partial}{\partial t}(\epsilon\rho)}_{\substack{\textit{rate of mass change}\\ \textit{per unit volume}}} + \underbrace{\nabla \cdot (\epsilon\rho\mathbf{U})}_{\substack{\textit{net rate of mass change}\\ \textit{per unit volume by convection}}} = 0$$

Computational Fuel Cell Dynamics(CFCD)

2. Momentum conservation

$$\frac{\partial}{\partial t}(\epsilon\rho\mathbf{U}) + \nabla\cdot(\epsilon\rho\mathbf{U}\mathbf{U}) = -\epsilon\nabla p + \nabla\cdot(\epsilon\zeta) + \frac{\epsilon^2\mu\mathbf{U}}{\kappa}$$

rate of momentum change per unit volume	*convection*	*net rate of momentum change per unit volume by*		
		pressure	*viscous friction*	*pore structure*

Computational Fuel Cell Dynamics(CFCD)

3. Species conservation

$$\frac{\partial}{\partial t}(\epsilon\rho X_i) \quad + \quad \nabla\cdot(\epsilon\rho\mathbf{U}X_i) \quad = \quad \nabla\cdot\mathbf{J}_i \quad + \quad S_i \quad (\mathrm{E}$$

rate of a species mass change per unit volume — *net rate of a species mass change per unit volume by* — *convection*, *diffusion*, *electrochemical reaction*

$$S_i = M_i\frac{j}{n_i F}$$

$$J_i = \rho D_{eff,j}\nabla X_i + \frac{\rho Y_i}{M} D_{eff,i}\nabla M - \rho M\sum_j D_{eff,j}\nabla Y_j - \rho\nabla M\sum_j D_{eff,j} Y_j$$

Computational Fuel Cell Dynamics(CFCD)

4. Charge conservation

$$\nabla \cdot \mathbf{i} = 0$$

$$\nabla \cdot \mathbf{i}_{elec} + \nabla \cdot \mathbf{i}_{ion} = 0$$

$$-\nabla \cdot \mathbf{i}_{ion} = \nabla \cdot \mathbf{i}_{elec} = j$$

$$\nabla \cdot (\sigma_{ion} \nabla \Phi_{ion}) = -\nabla \cdot (\sigma_{elec} \nabla \Phi_{elec}) = j$$

$$j = j_0 \exp\{\frac{n_i \alpha F}{RT}(\Phi_{ion} - \Phi_{elec})\}\frac{c_i}{c_i^0}$$

Computational Fuel Cell Dynamics(CFCD)

5. Energy conservation

$$\frac{\partial}{\partial t}(\varepsilon\rho h)+\nabla\bullet(\varepsilon\rho\mathbf{U}h)=\nabla\bullet\mathbf{q}+\varepsilon\boldsymbol{\tau}:\nabla\mathbf{U}+\varepsilon\frac{\mathrm{d}p}{\mathrm{d}t}-j_T\eta+\frac{\mathbf{i}\bullet\mathbf{i}}{\sigma}+\dot{S}_h$$

$$\mathbf{q}=k_{eff}\nabla T+\sum_{k=gas}\mathbf{J}_k h_k$$