The optimal electrode thickness and porosity

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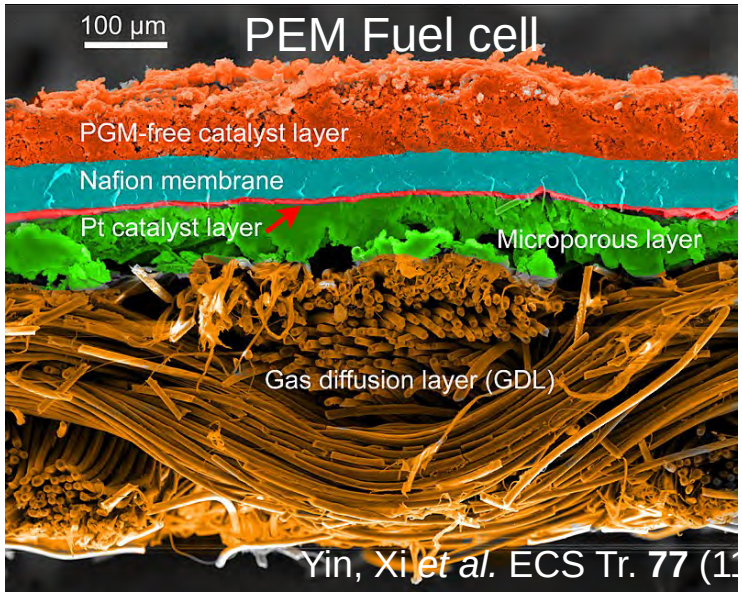
Process & energy

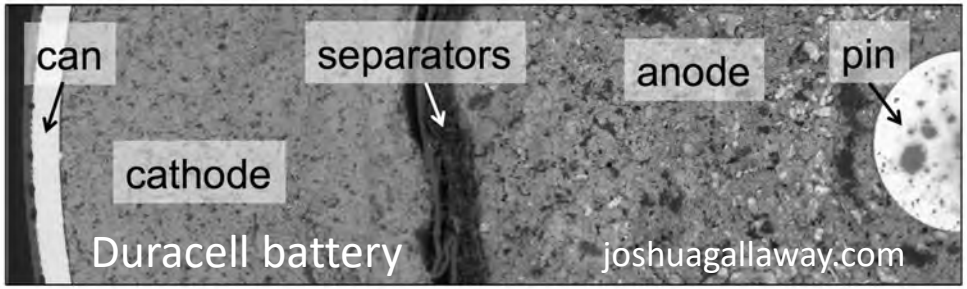
e-Refinery

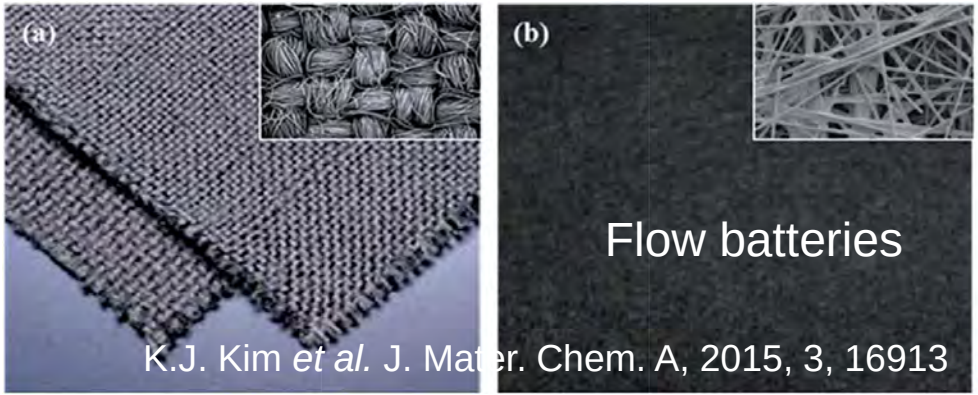
Towards sustainable production of chemicals and fuels

TU Delft

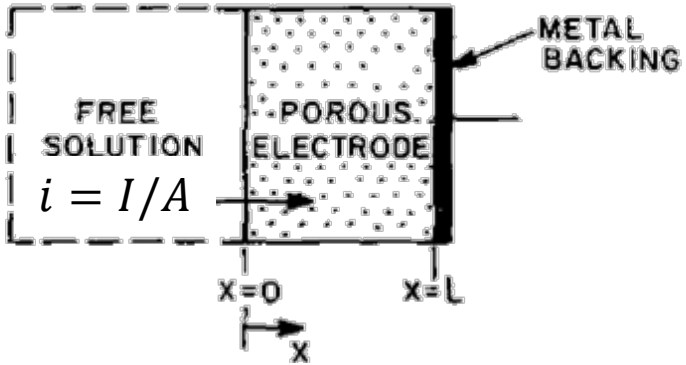
Porous electrodes



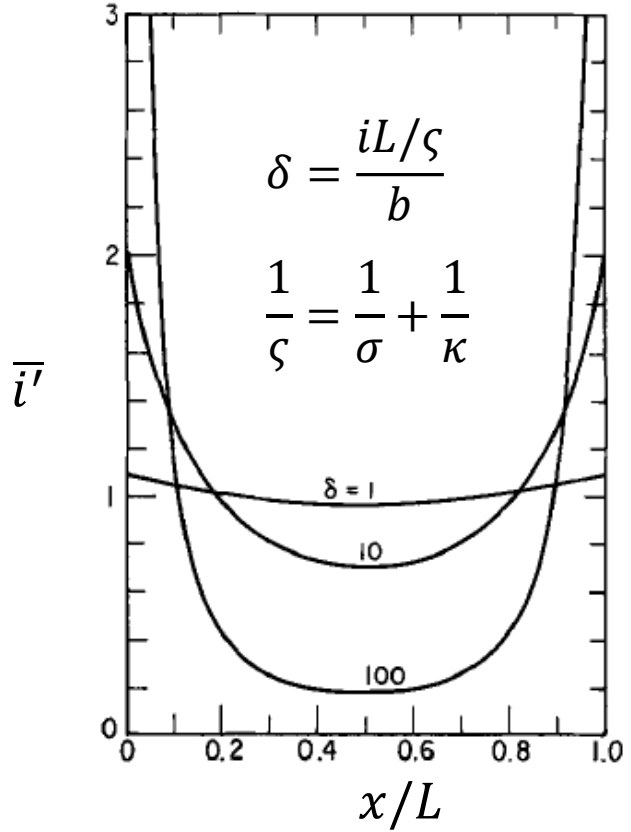




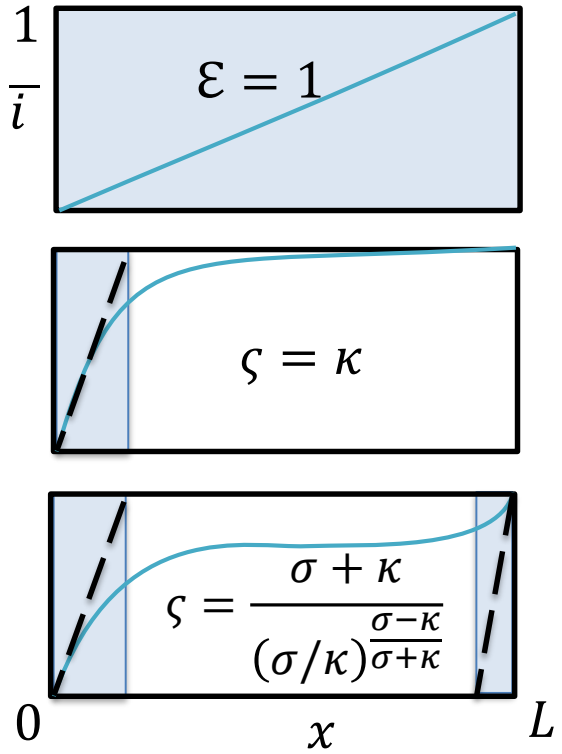
Newman & Tobias 1962



- Constant conductivities σ, κ
- Tafel slope $b = RT/\alpha F$



Electrode *Effectiveness Factor*



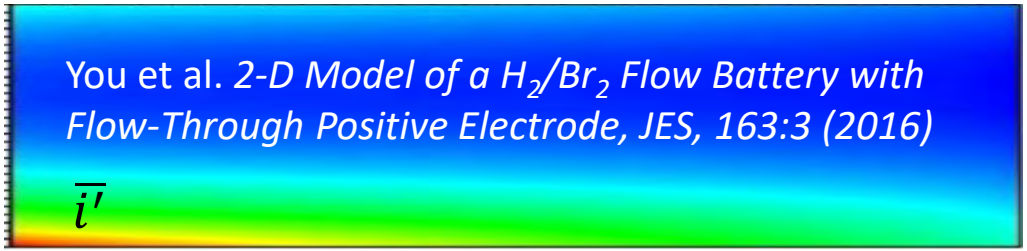
$$\Delta V = b \ln\left(\frac{i}{\varepsilon i_*^{\mathrm{tot}}}\right) + \frac{iL}{\sigma + \kappa}$$

$$i_*^{\mathrm{tot}} = aLi_*$$

$$\varepsilon \approx (1 + \mathcal{I}^p)^{-\frac{1}{p}}$$

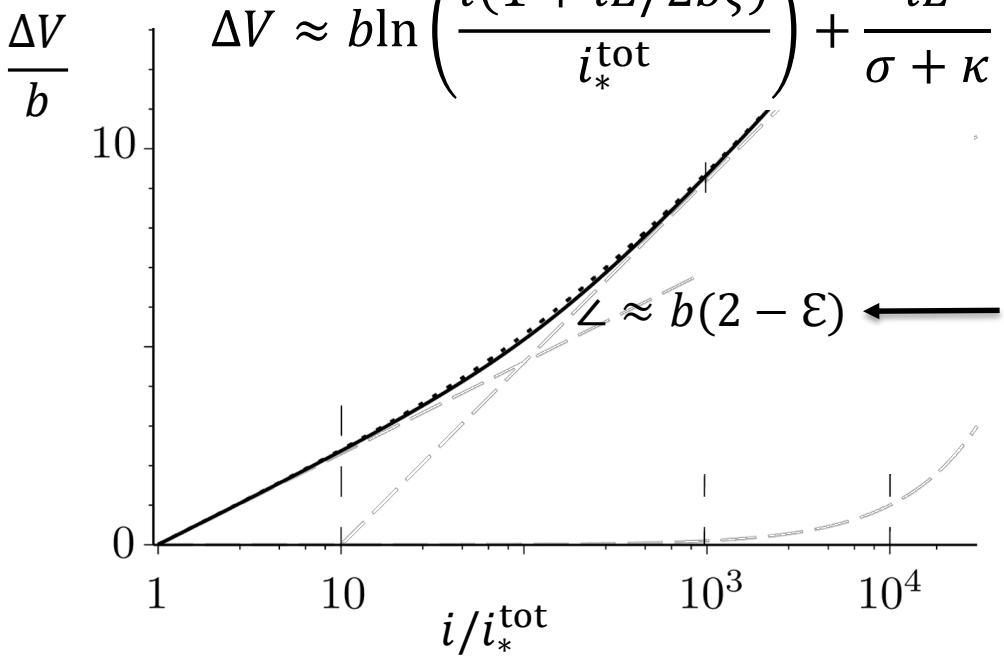
$$\mathcal{I} \sim \delta/2$$

Paulin *et al.* '77, Scott '82, Costamagna *et al.*, '98
C*atalyst utilization*, e.g. Gasteiger *et al.*



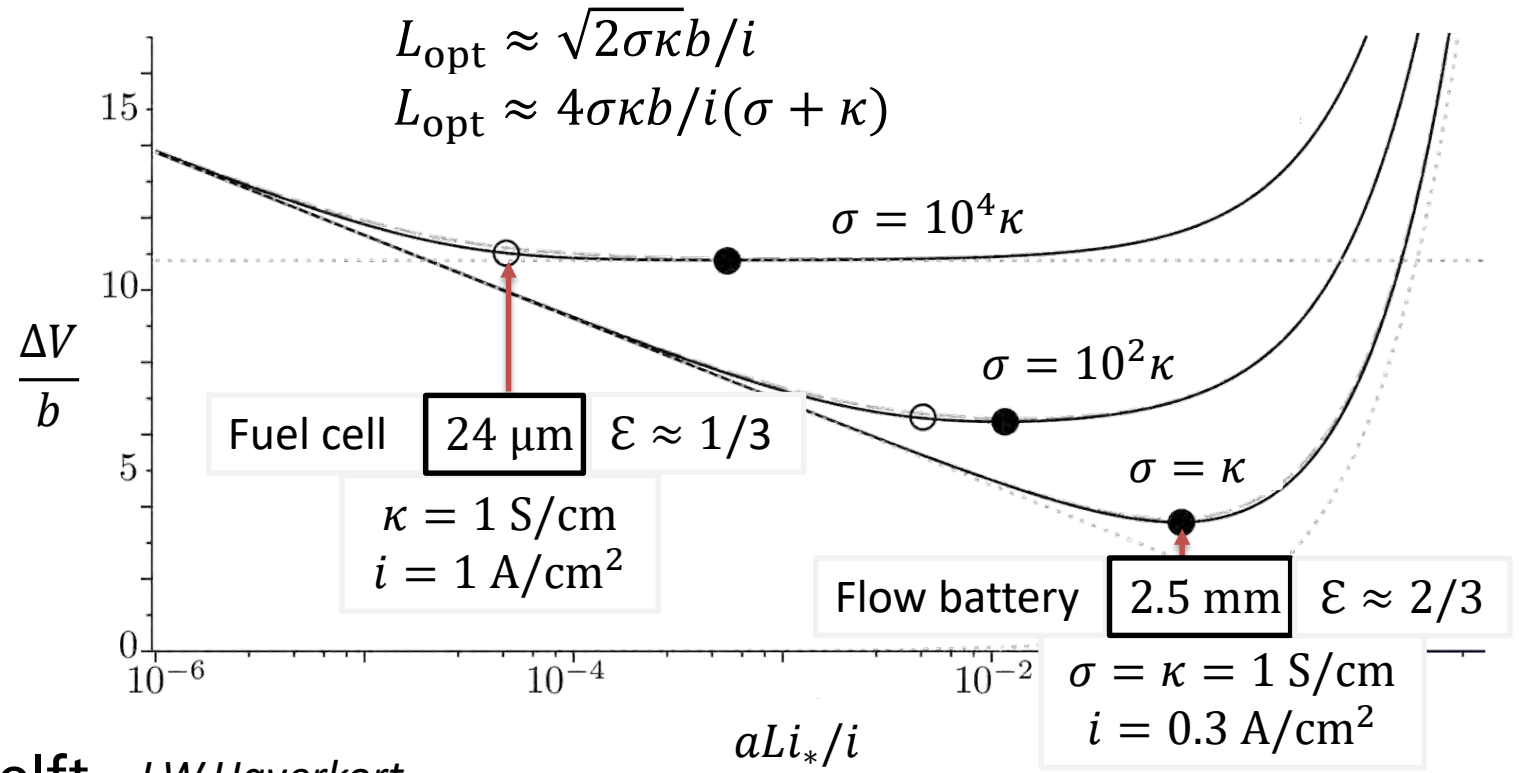
Explicit $i - \Delta V$ relation

$$\Delta V \approx b \ln\left(\frac{i(1 + iL/2b\varsigma)}{i_*^{\mathrm{tot}}}\right) + \frac{iL}{\sigma + \kappa}$$



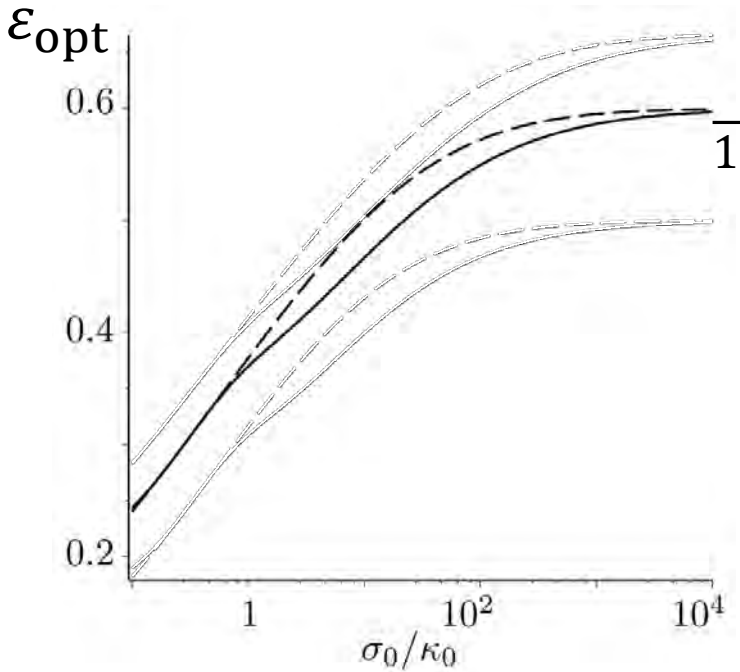
Tafel slope doubling
Austin, Eikerling, Kulikovsky, Soderberg,..

Optimal electrode thickness

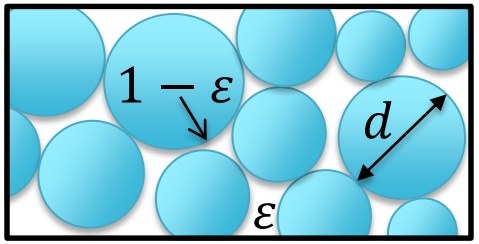


Optimal porosity

$$\kappa = \kappa_0 \varepsilon^{1.5}, \sigma = \sigma_0 (1-\varepsilon)^{1.5}$$

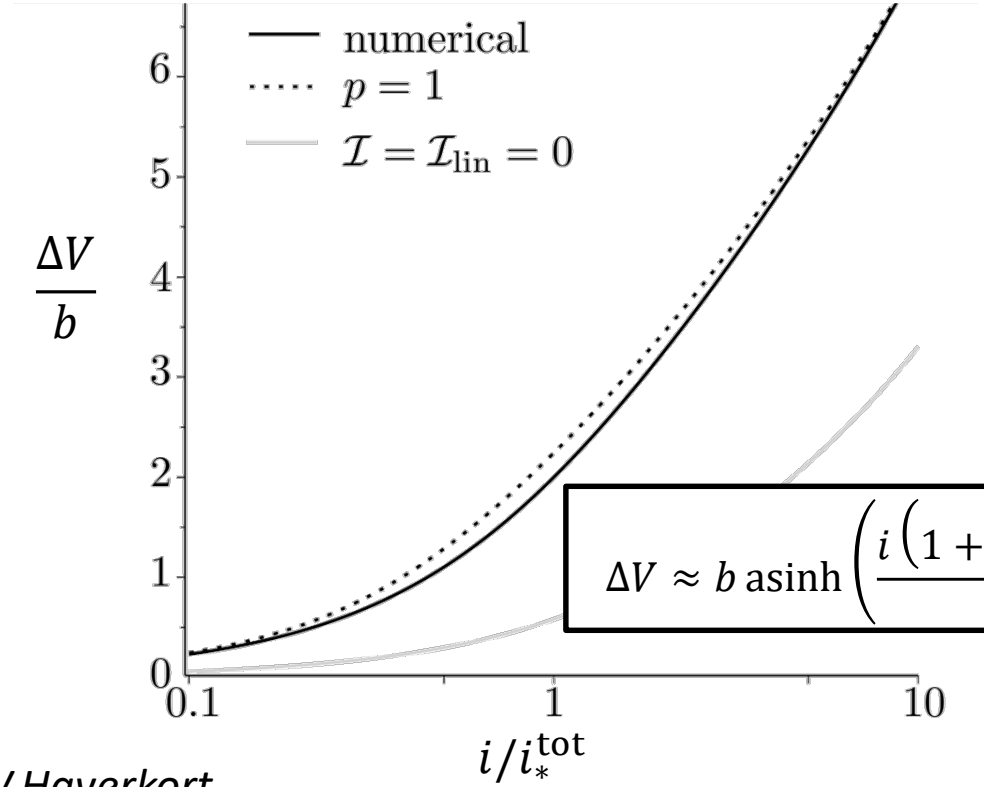


$$\frac{1.5}{1+1.5} = 0.6$$



$$a = \frac{6(1-\varepsilon)}{d}$$

Butler-Volmer kinetics (α=1/2)



$$\Delta V \approx b \,\text{asinh}\left(\frac{i\left(1+\left(\mathcal{I}^p+\mathcal{I}_{\text{lin}}^p\right)^{\frac{1}{p}}\right)}{2i_*^{\text{tot}}}\right)+\frac{iL}{\sigma+\kappa}$$

Conclusions

- Tafel slope $b(2-\mathcal{E})$
- Thickness $L_{\mathrm{opt}} \approx \frac{4b\sigma\kappa}{i(\sigma+\kappa)}$ so that $\frac{1}{3} \leq \mathcal{E} \leq \frac{2}{3}$
- Accurate *explicit* polarisation equation

Haverkort, J. W. (2019). *Electrochimica Acta*, *295*, 846-860.
A theoretical analysis of the optimal electrode thickness and porosity.

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