RESULTS

The model evaluated the time dependent and...

METHODOLOGY

The model is based on the short term metathesis and offers...

ACKNOWLEDGMENTS

I extend the authorship of this work to...

METHODS

The model overcomes the transition...

MATERIALS

The model is based on the short term metathesis and offers...

CONCLUSION

The model overcomes the transition...

REFERENCES

The model overcomes the transition...

APPENDIX

The model overcomes the transition...
modular design of simulation process
modeling approach of electrode on cathode side

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water removal rate

\[ \dot{V}_{\text{air}, \text{H}, \text{H}_2\text{O}, T, \text{backing, flow-field}} \]

\[ \text{e.g.} \quad J_{\text{H}_2\text{O}} = c_{\text{H}_2\text{O}} \cdot 3 \cdot (\phi_{\text{H}_2\text{O}} - \phi_{\text{H}_2\text{O}}) \]
modeling approach of electrode on anode side
modeling of mass transport in reactive layers

gas-phase species
\[
- \frac{d p_i}{d z} - p_i \frac{B_0}{\eta_g D_j^g} \frac{d p}{d z} = R T \left( \frac{J_j^g}{\tau_g D_j^g} \right) + \sum_{i: i \neq j}^{K} \frac{p_i J_j^g - p_j J_i^g}{p_i \tau_g D_{ij}^g},
\]

liquid water
\[
J^l_w = - \frac{\varepsilon_i}{\tau_l} \frac{D_i}{D_w} \frac{d c_w}{d z} + \frac{3}{F} i_{H^-}.
\]
dissolved methanol
\[
J^l_m = - \frac{\varepsilon_i}{\tau_l} \frac{D_i}{D_m} \frac{d c_m}{d z} + \frac{c_m}{55.56} J^l_w.
\]
modeling of electrochemical reactions

reaction rate of oxygen reduction

\[ j_1 = -a_1 i_1^{ref} \exp\left(\frac{-E_{o1}^c}{R} \left(\frac{1}{T} - \frac{1}{T_{ref}}\right)\right) \frac{c_{O_2}}{c_{O_2}^{ref}} \exp\left(\frac{2.3\eta_1}{b_1}\right) \]

reaction rate of methanol oxidation

\[ j_2 = a_2 i_2^{ref} \exp\left(\frac{-E_{o2}^c}{R} \left(\frac{1}{T} - \frac{1}{T_{ref}}\right)\right) \frac{c_m}{c_{m}^{ref}} \exp\left(\frac{2.3\eta_2}{b_2}\right) \]

gradient of ionic current density

\[ \frac{di_{i^+}}{dz} = j_1 - j_2 \]
cathode performance - experiment / simulation

(4mgcm\(^2\) Pt. 90°C. 20psig air, 1 l/min)
average volume fraction of gas pores in cathodic reaction layer

volume fraction of through pores / %

current density / mA cm^-2

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Distribution of reaction rate in cathodic reaction layer

reaction rate / Am$^{-3}$

position in reaction layer / $\mu$m

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Distribution of oxygen concentration in cathodic reaction layer

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anode performance - experiment / simulation
(12 mg/cm$^2$ Pt-Ru, 1 M MeOH, 90°C)
Distribution of reaction rate in anodic reaction layer

![Graph showing the distribution of reaction rate in anodic reaction layer with different current densities and position in reaction layer. The x-axis represents the position in reaction layer (μm) and the y-axis represents the reaction rate (Am⁻³).](chart.png)
Distribution of ionic current density in anodic reaction layer
Distributio\n of methanol concentration in anodic reaction layer

\[ \text{methanol concentration (mol/l)} \]

\[ \text{position in reaction layer (\( \mu \text{m} \))} \]
effect of anodic reaction layer thickness on methanol crossover

- $6 \times 10^{-6}$
- $4 \times 10^{-6}$
- $2 \times 10^{-6}$

- $12 \text{mgcm}^{-2} \text{Pt-Ru}$ (experimental data)
- $4 \text{mgcm}^{-2} \text{Pt-Ru}$ (experimental data)
- simulation result

methanol crossover / kmolm$^{-2}$s$^{-1}$

current density / mAcm$^{-2}$
effect of anodic reaction layer thickness on anode potential at 500 mA cm$^{-2}$

- catalyst-loading-thickness
- catalyst-loading=const=12 mg cm$^{-2}$

Electrode potential / V vs. thickness of reaction layer / μm
effect of anodic reaction layer thickness on anode potential at 250 mAcm$^{-2}$
fraction of migration compared to total methanol crossover rate in Nafion 117 at 90°C
methanol crossover - effect of driving forces

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effect of methanol crossover on cell performance

(1M MeOH, 90°C, 20psig air, 5l/min)
simulation result of cell performance at 90°C, 20psig air separation into individual electrode potentials