Detailed Electrochemical and Fluid Modelling of SOFC Relating Gas Distribution to Cell Degradation

Engine Expo 2008

07.05.2008

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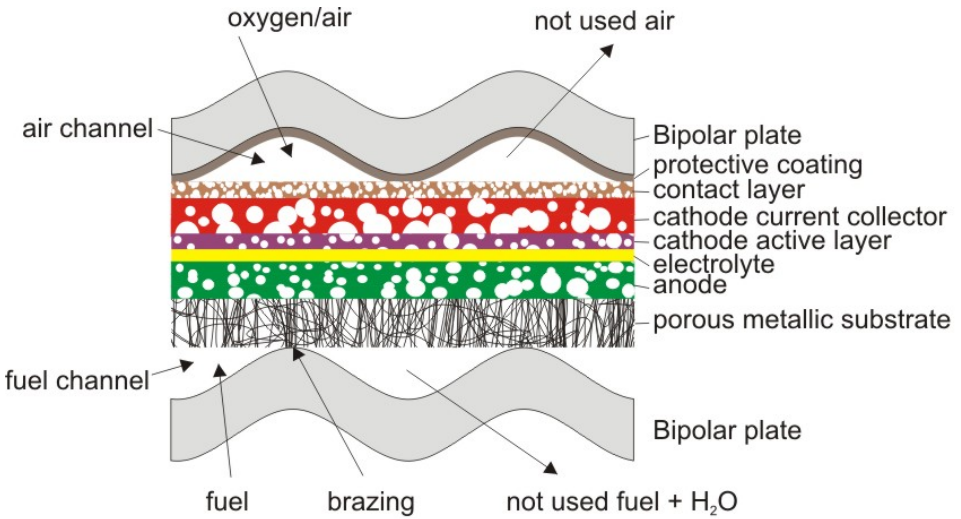
Overview

- Introduction
  - Solid Oxide Fuel Cells (SOFC)
  - Cell and Diffusion Polarisation
  - CFD Modelling
  - Degradation
- Model of a small Segment of SOFC
- Modelling Results
- Comparison with Measurements
- Conclusion

Introduction – Solid Oxide Fuel Cell (SOFC)

- Operating temperature 600°C – 1000°C
- Reaction takes place at porous electrodes – electrolyte interface
- Fabrication with Sintering or Vacuum Plasma Spray Technology (VPS)

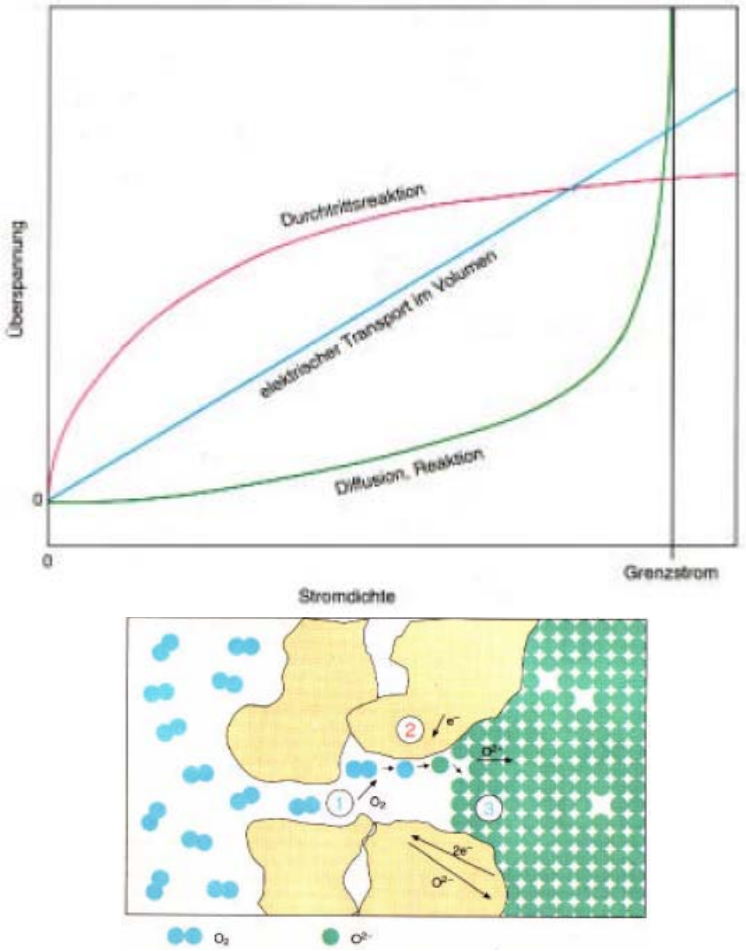


(not in scale)

Introduction – Cell and Diffusion Polarisation

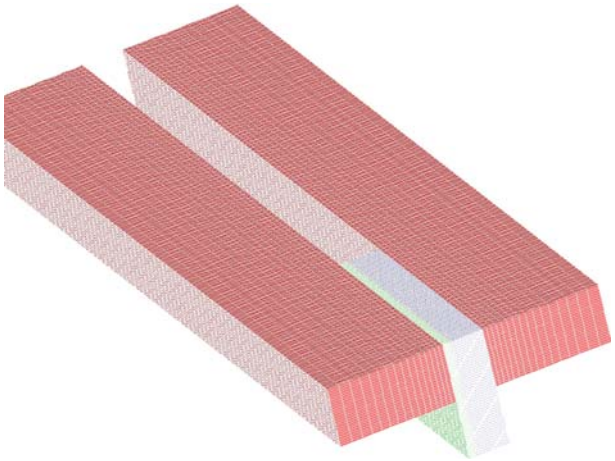
- Nonlinear behaviour of the U-I-Characteristics forced by increase of diffusion polarisation reaching the maximum current density

- Because of the low gas diffusion velocity of the educts the demanded amount cannot be converted



Introduction – CFD Modelling

- Use of the commercial software package “Star-CD” from cd-adapco
- Conservation equations for mass, impulse and energy are solved in parallel
- Mapping of flow field and porous electrodes
- Two-dimensional electrochemical approach
- Implementation of different user-subroutines:
  - For electrochemistry
  - For mass transfer from cathode to anode
  - For surface reactions
  - For user-defined gas diffusion coefficients



Introduction - Degradation

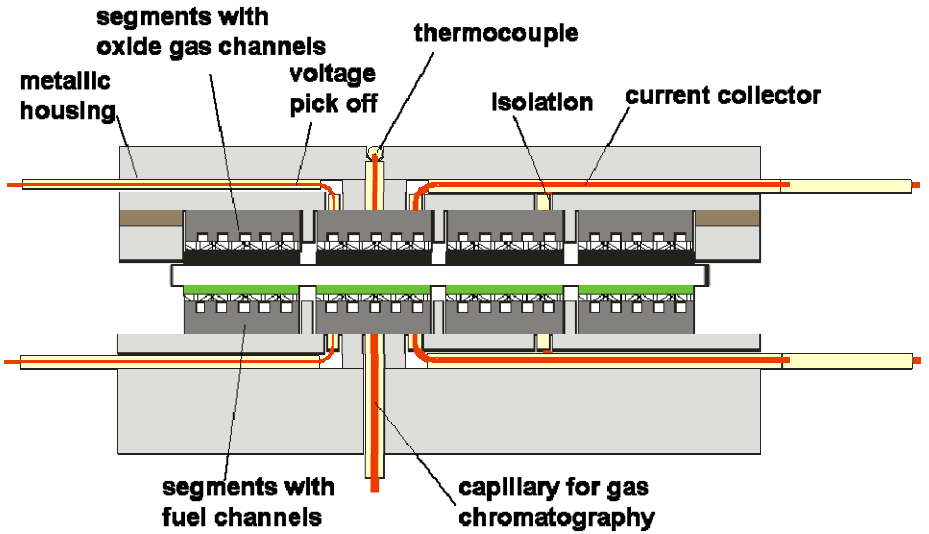
Degradation in SOFC could be caused by:

- Inter-material diffusion, separation of compound materials
- Blocking of active zones by pollutants
- Metal sintering during operation and decrease in porosity
- Evaporation of Nickel in the Anode

- Electrochemical processes because of lack of educts?

Electrochemical Model from Measurements

- Measurements with segmented cell geometry
- Measurement of cell temperature and local gas concentrations
- Measurement of polarisations and impedance
- Development of a temperature and concentration depending electrochemical model



(Dissertation P.Metzger; Diplomarbeit T.Franke, DLR TT)

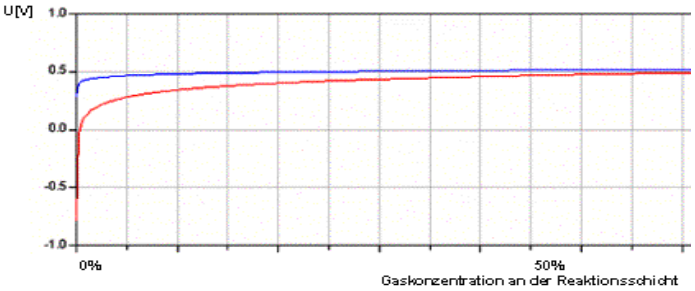
Electrochemical Model from Measurements

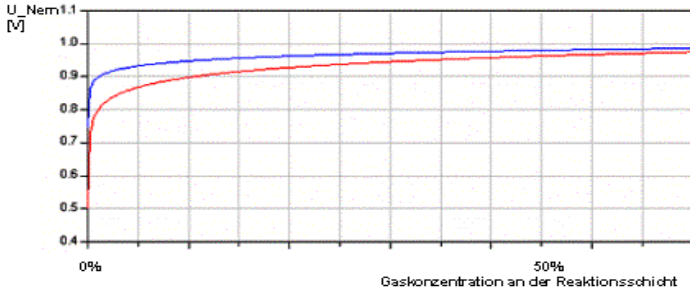
$$U = U_{Nernst} - \eta_{Ohm} - \eta_{Pol}$$

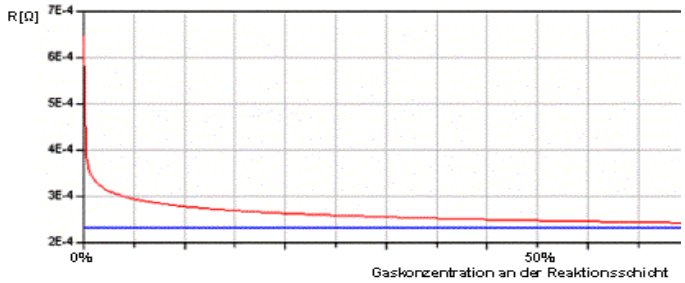
$$U_{Nernst} = -\frac{\Delta G}{zF} + \frac{RT}{zF}\ln\left(\frac{(p_{O_2}/p_{ges})^{0,5}(p_{H_2}/p_{ges})}{(p_{H_2O}/p_{ges})}\right)$$

$$\eta_{Ohm} = C_1 e^{\frac{C_2}{T}} \cdot i \qquad \eta_{Pol} = C_3 e^{-\left(C_4 \ln\left(\frac{p_{H_2}}{p_{ges}}\right)\right)} \cdot i$$

(Dissertation P.Metzger; Diplomarbeit T.Franke)



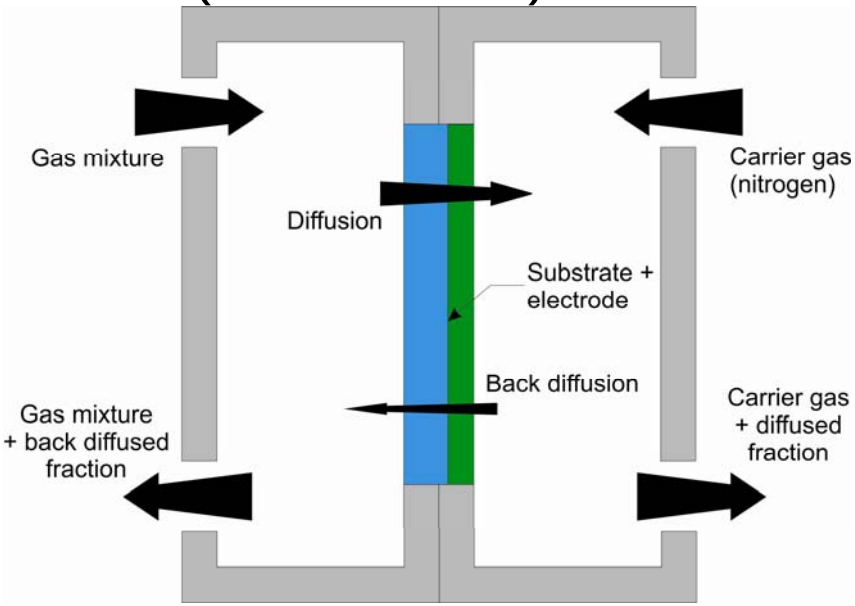




Measurement of Gas Diffusion Coefficients

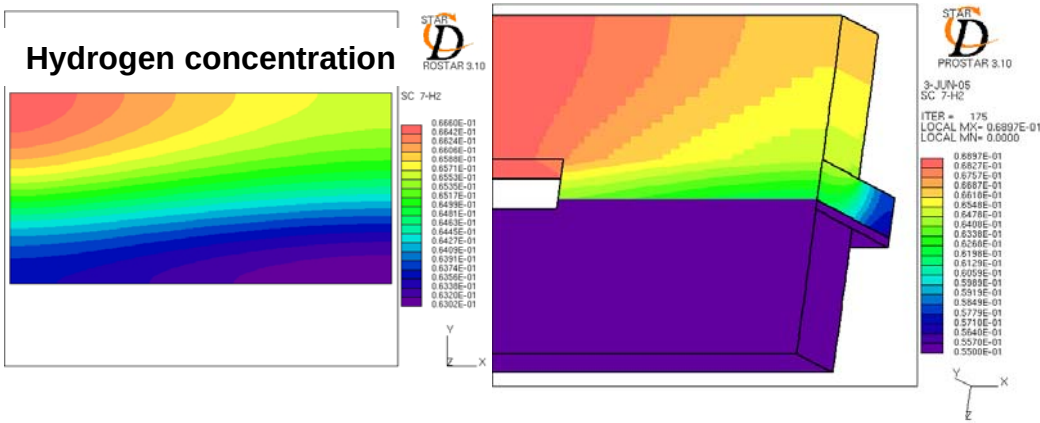
Measurement of effective gas diffusion coefficients:

- In the porous electrodes
- In the relevant temperature regime (up to 900 °C)
- Of mixtures of fuel cell gases in carrier gas (nitrogen)
- In the relevant range of concentrations (5 % to 50 %)

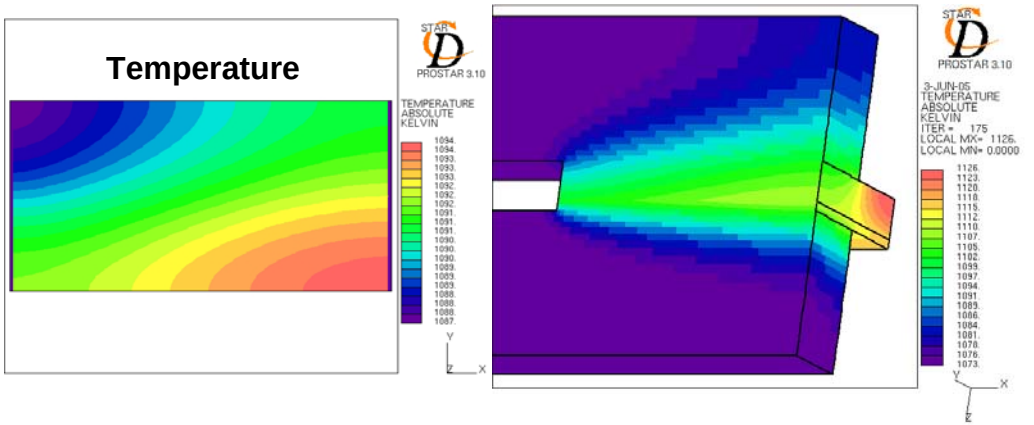


Results – Linear Regime

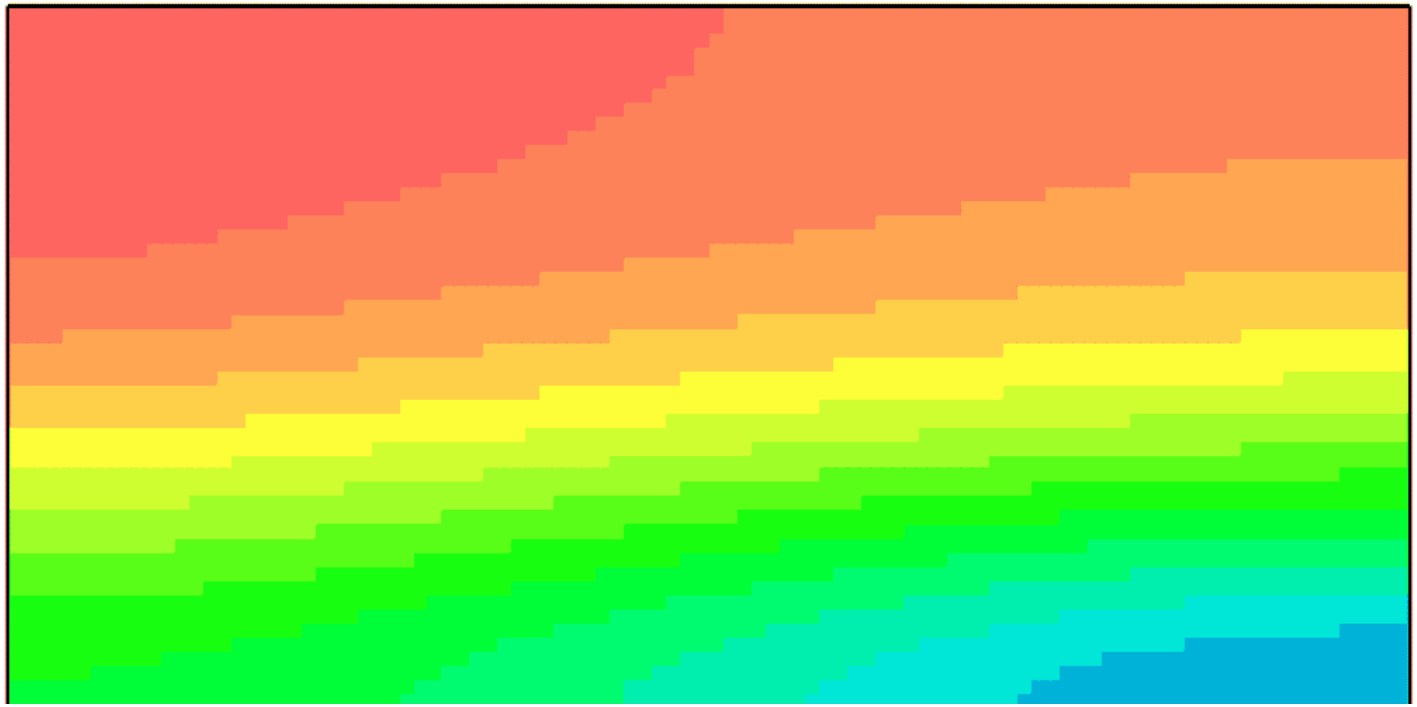
- 3-D concentration distribution of the educts in the linear regime of the characteristics



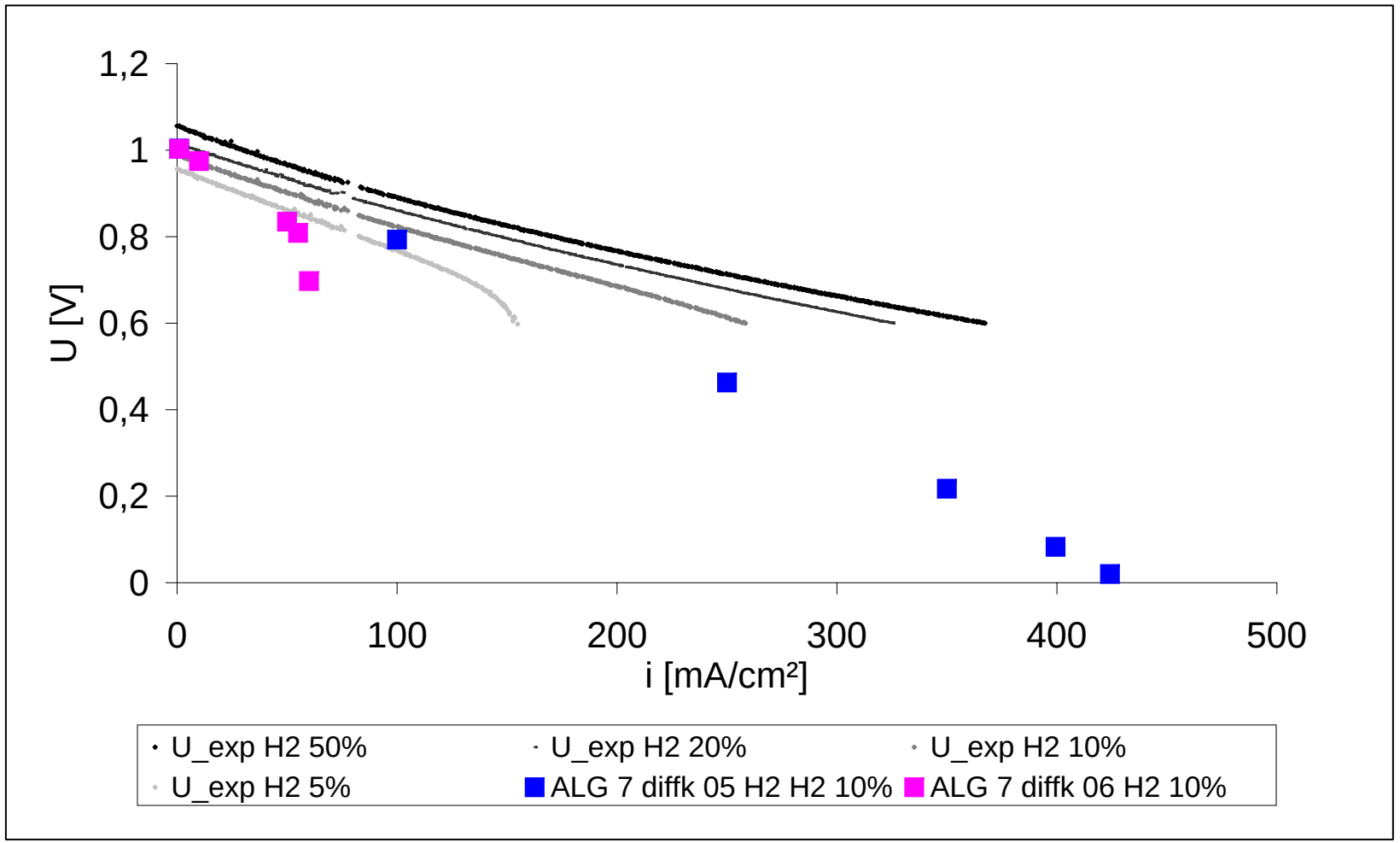
- Temperature distribution in the linear regime



Results – Conversion Rate



Results – Comparison with Measurements



Conclusion

- Diffusion polarisation represented by flow field
- Influence of the flow field to the electrochemistry
- Degradation effects identified
- Local degradation effects occurring at lower power densities than displayed in characteristics

- The developed model is able to evaluate flow field and cell geometry at different operating conditions

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