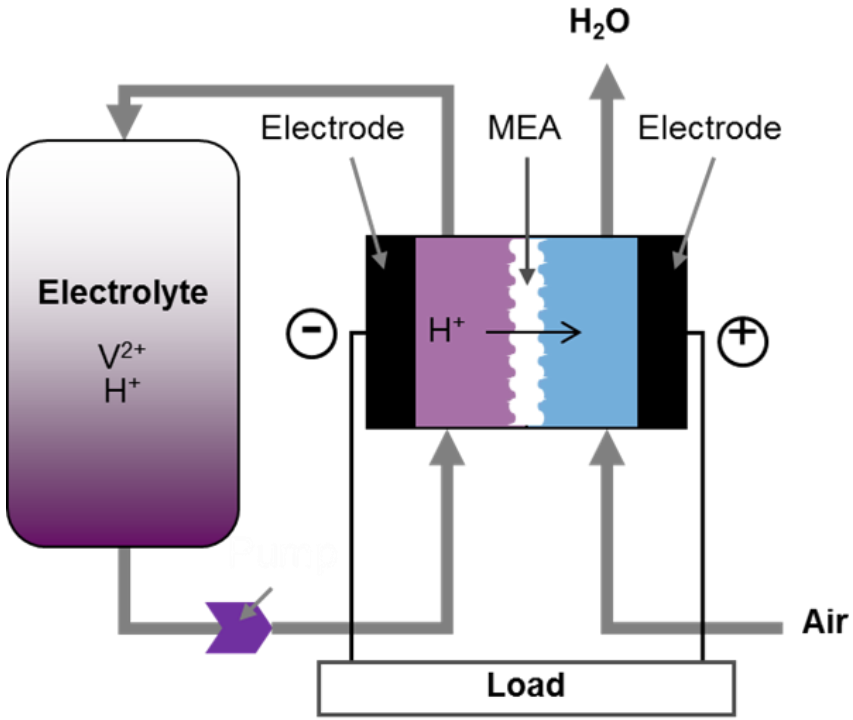
Modeling the Vanadium Oxygen Fuel Cell

F.T. Wandschneider, M. Küttinger, P. Fischer, K. Pinkwart, J. Tübke, H. Nirschl



COMSOL CONFERENCE ROTTERDAM2013

Fraunhofer ICT

Contents

Vanadium Redox Flow Battery

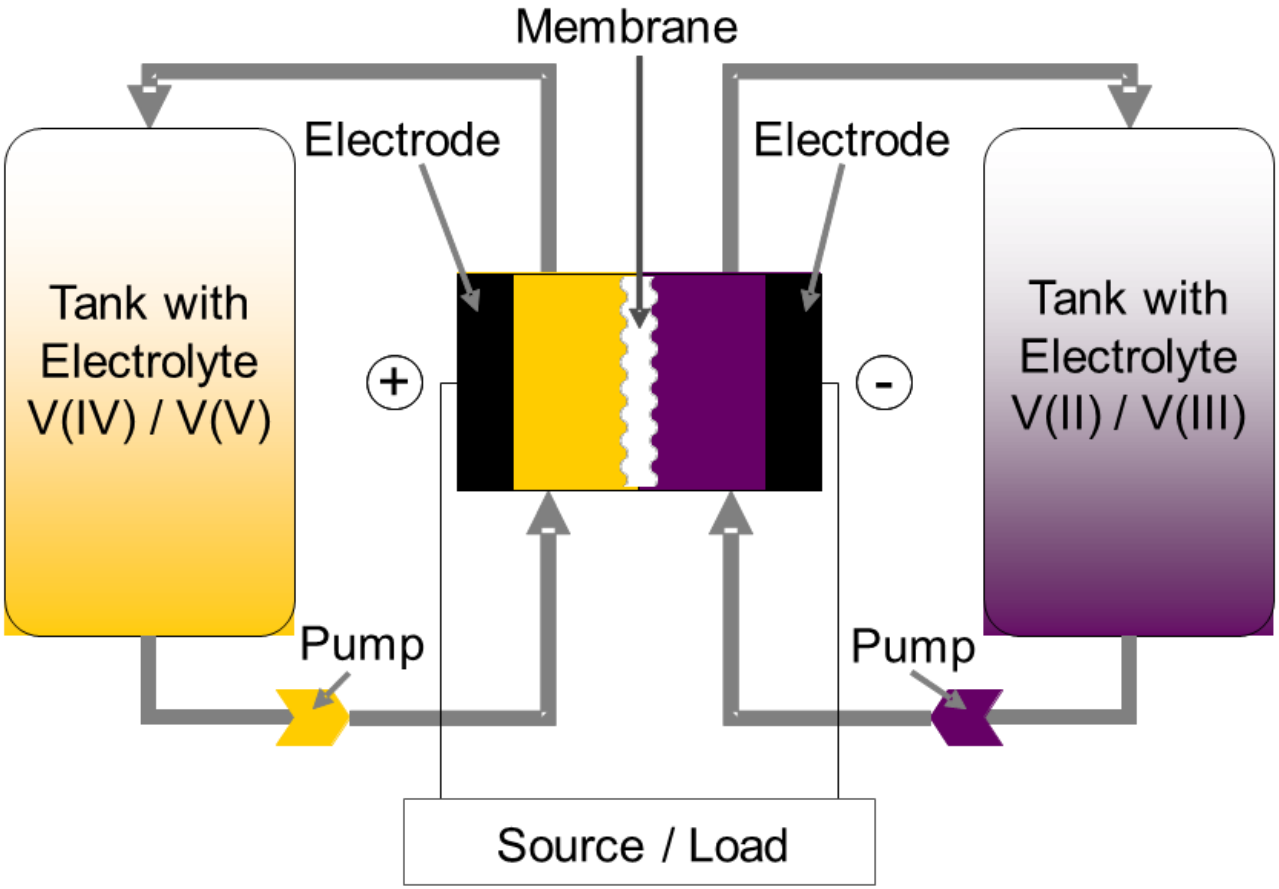
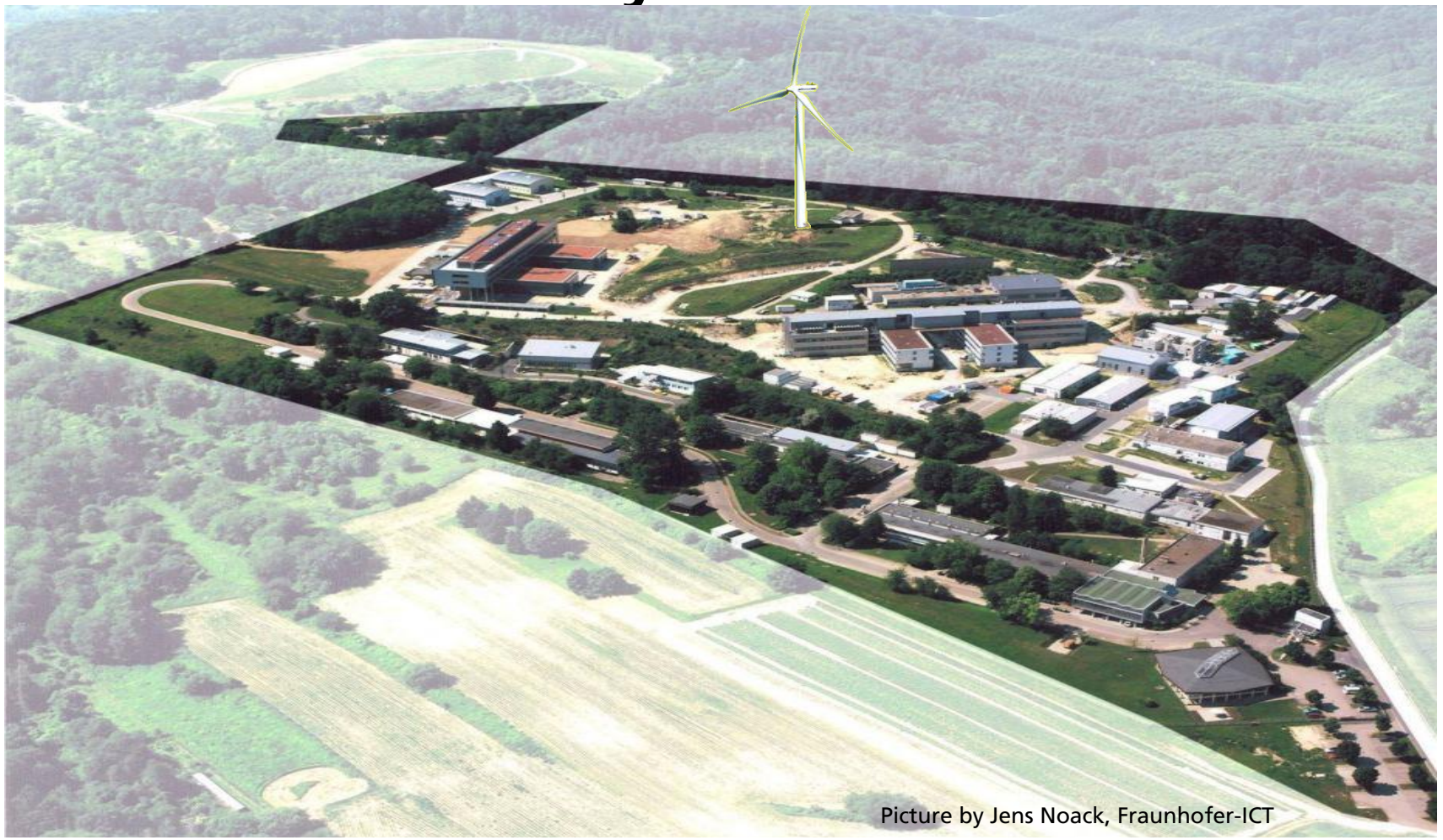


Figure by Jens Noack, Fraunhofer-ICT

Fraunhofer ICT

Project work: Planned 2 MW / 20 MWh Redox Flow Battery at our Institute



Fraunhofer ICT

Vanadium Air Redox Flow Battery

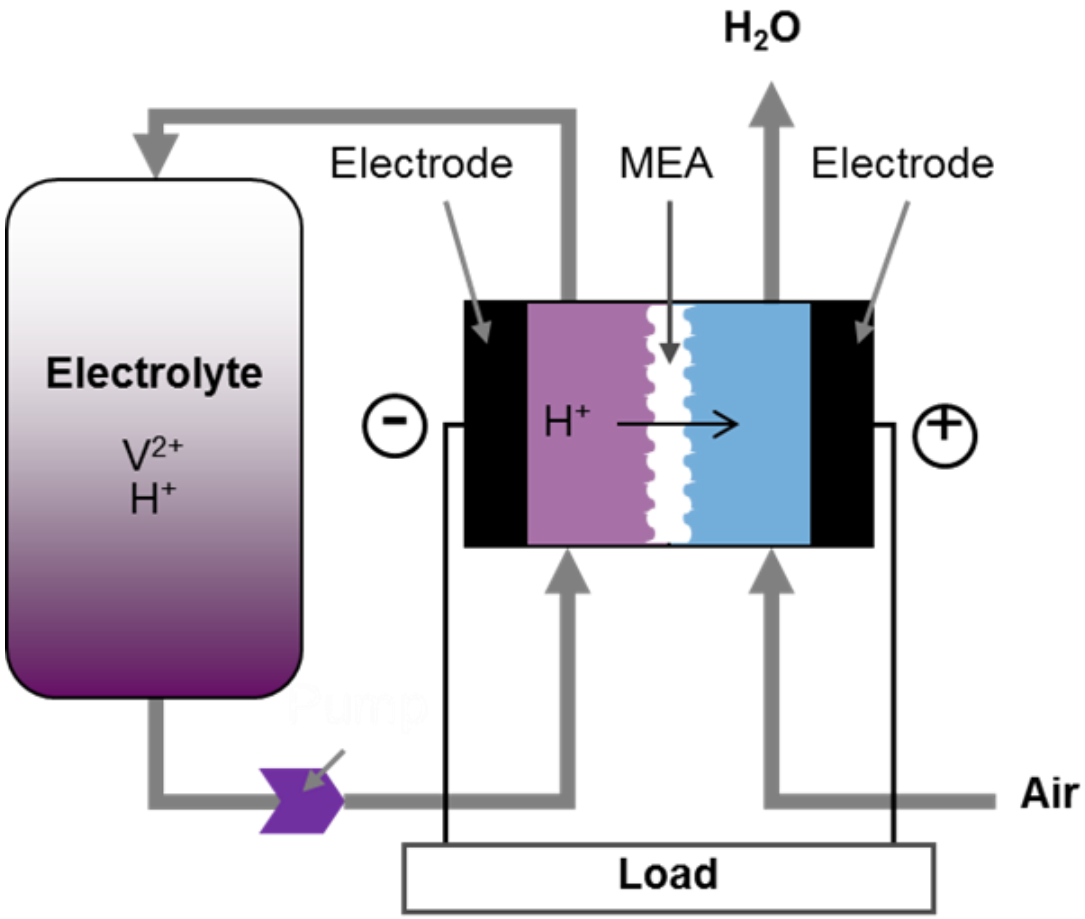
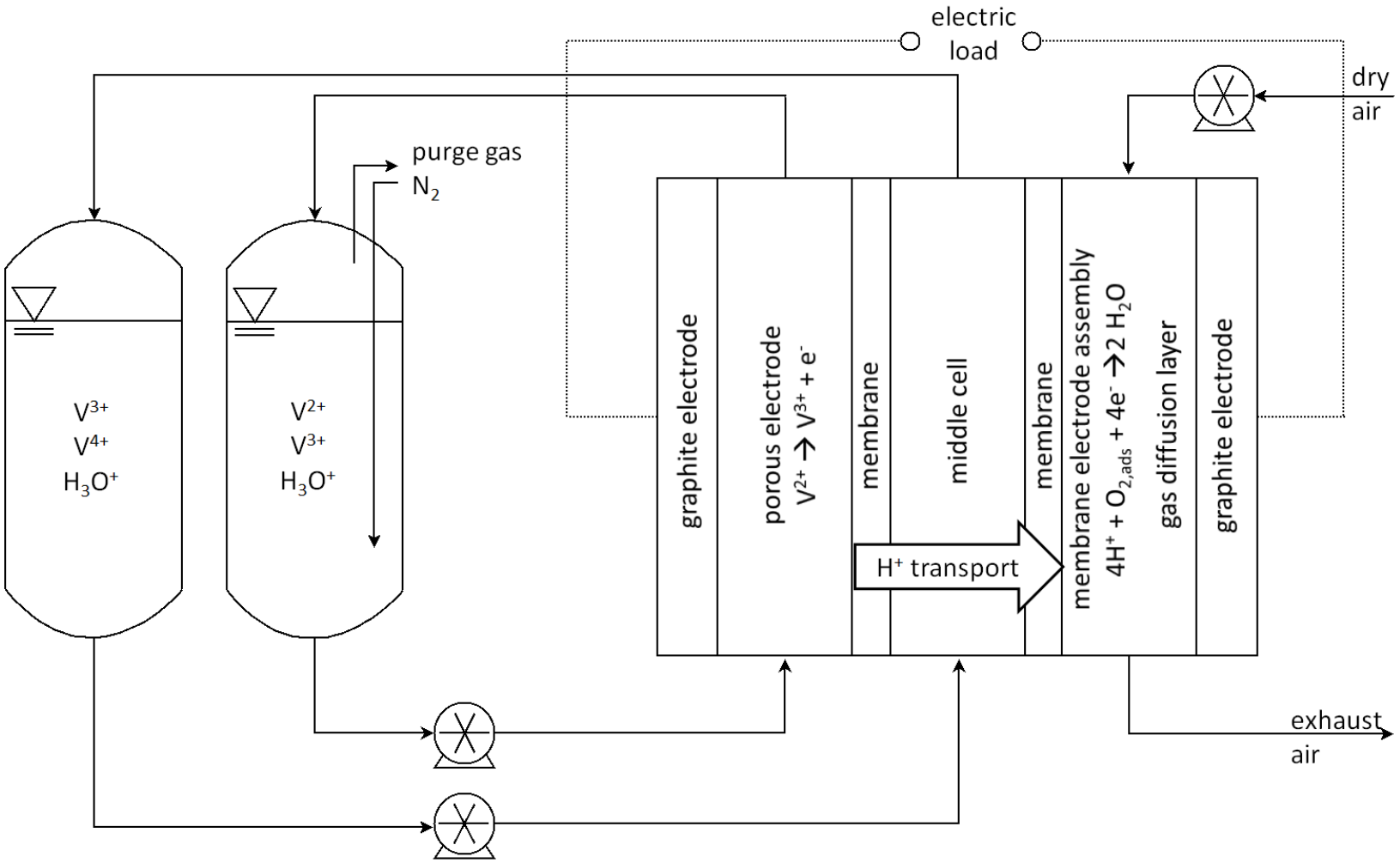


Figure by Jens Noack, Fraunhofer-ICT

Fraunhofer ICT

Vanadium Oxygen Fuel Cell

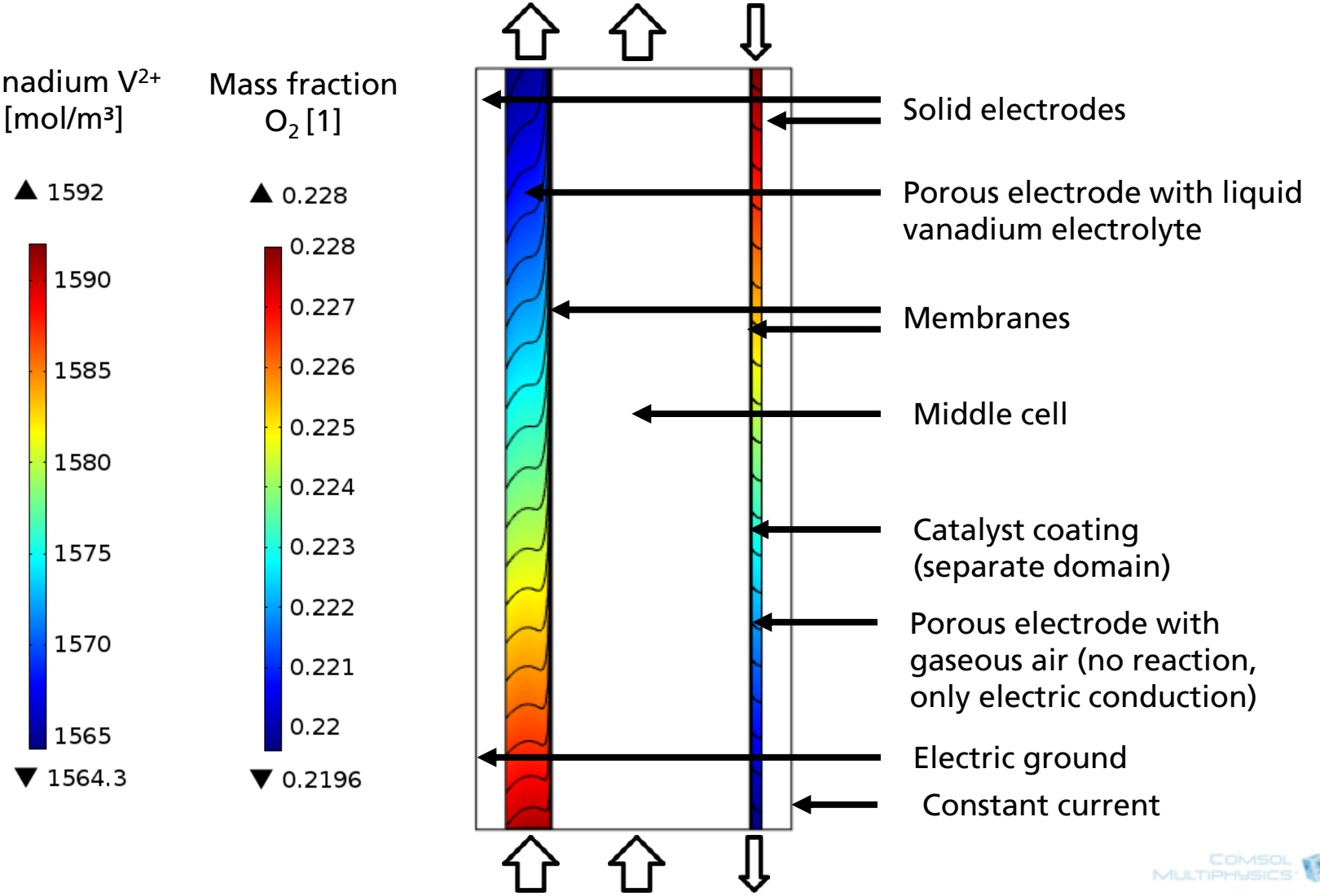


Fraunhofer ICT

Multiphysics Modeling

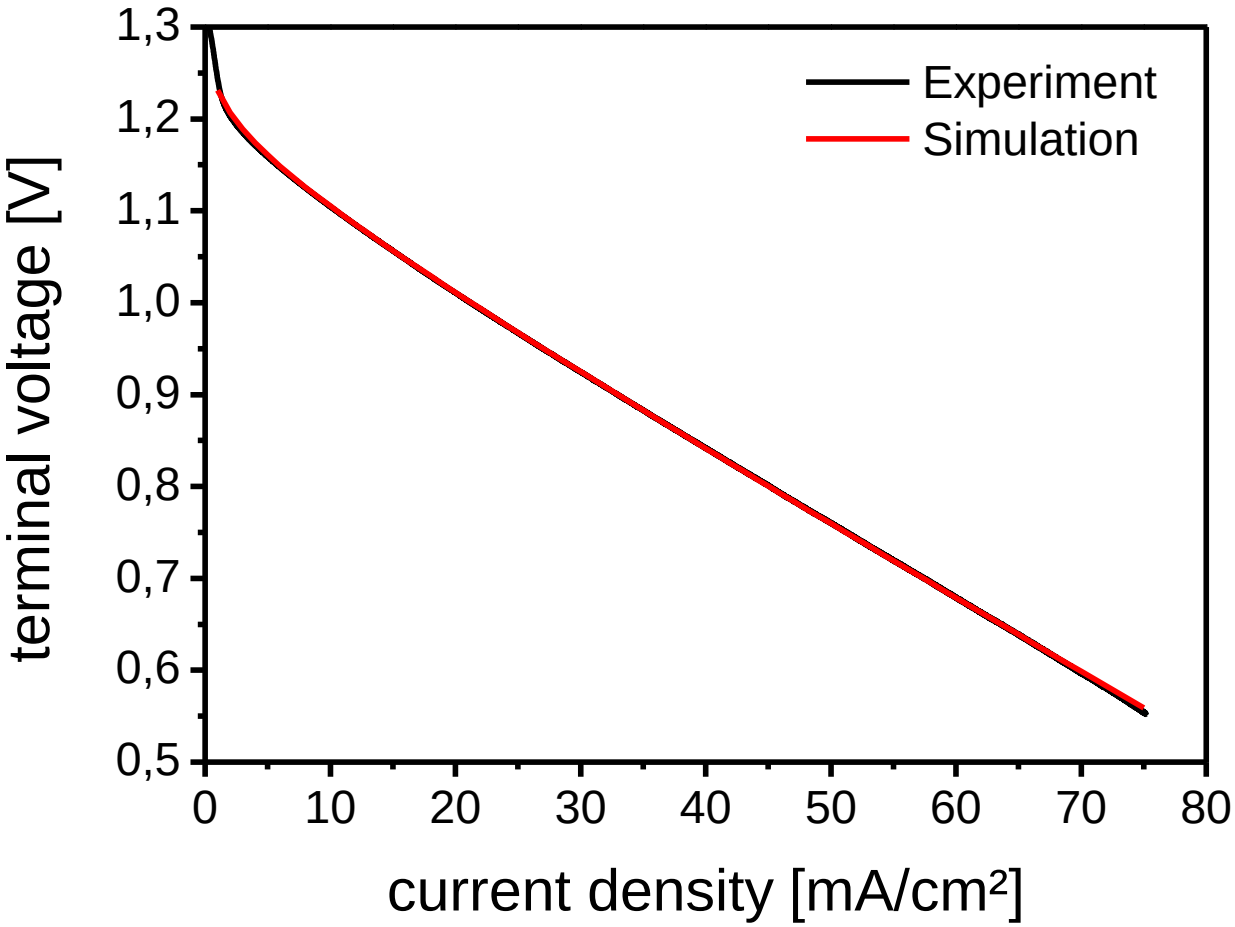
- Momentum
  - Liquid flow in vanadium half-cell and middle cell (porous media flow)
  - Gaseous flow in air half-cell
- Mass and species
  - Diluted species in vanadium half-cell and middle cell
  - Concentrated species in air half-cell
- Chemical reaction
  - „Bulk“ reaction within the porous electrode of the vanadium half-cell
  - Reaction at the membrane surface within the air half-cell
- Electrochemistry
  - Local potentials depending on species concentration
  - Electric and ionic currents

Stationary Simulation (1)



Fraunhofer ICT

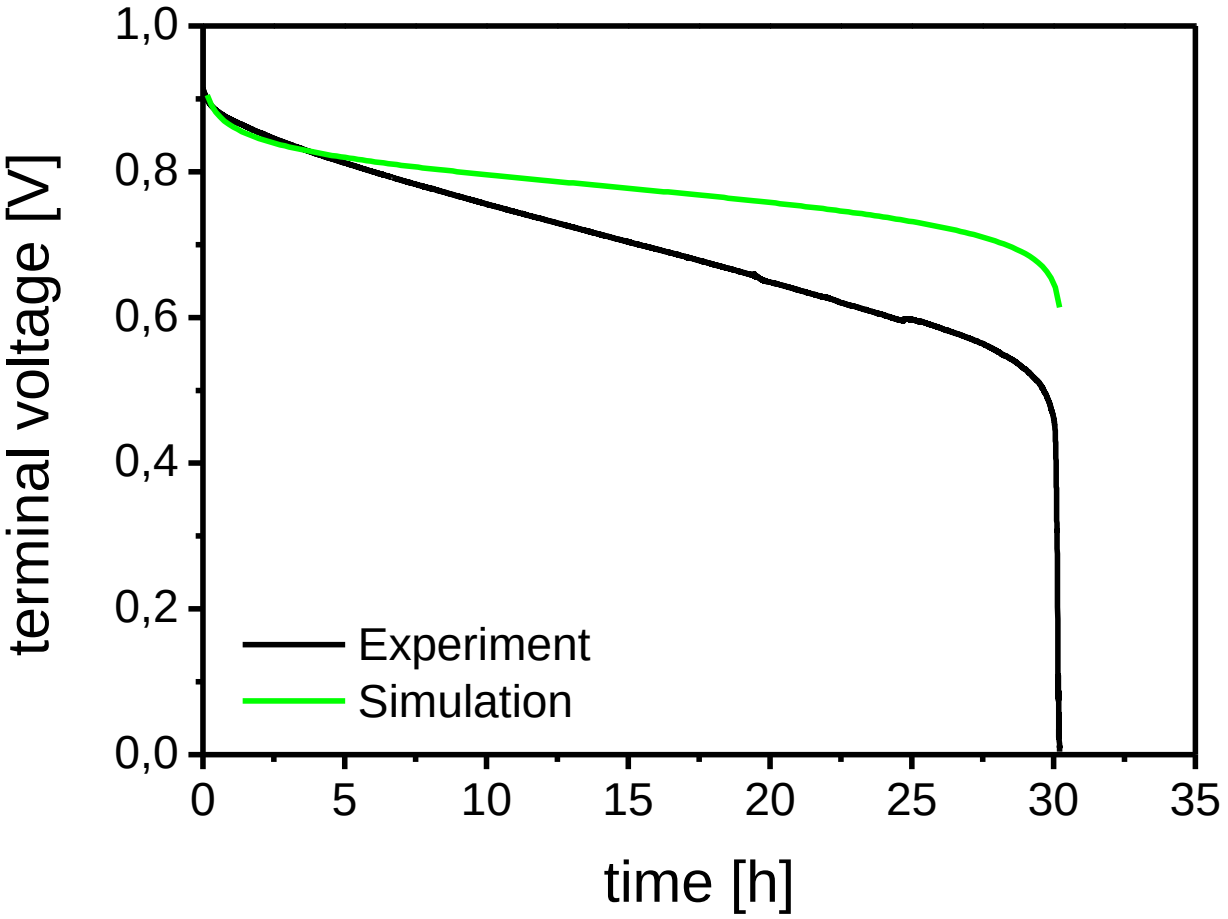
Stationary simulation (2)



Fraunhofer ICT

Time-dependent simulation

Discharge cycle with a constant current density of 25 mA/cm²

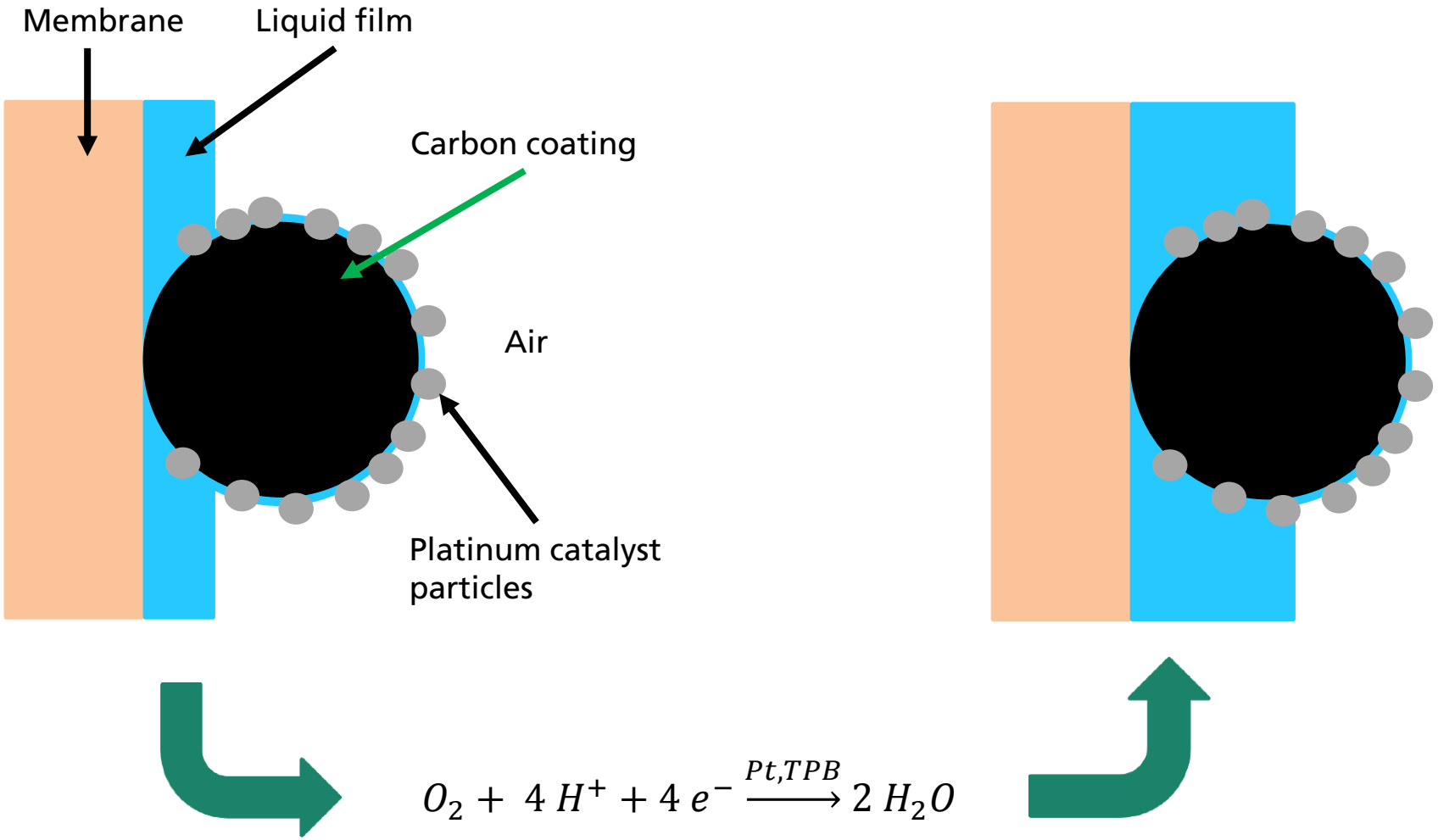


Fraunhofer ICT

Expanding the stationary model (1)

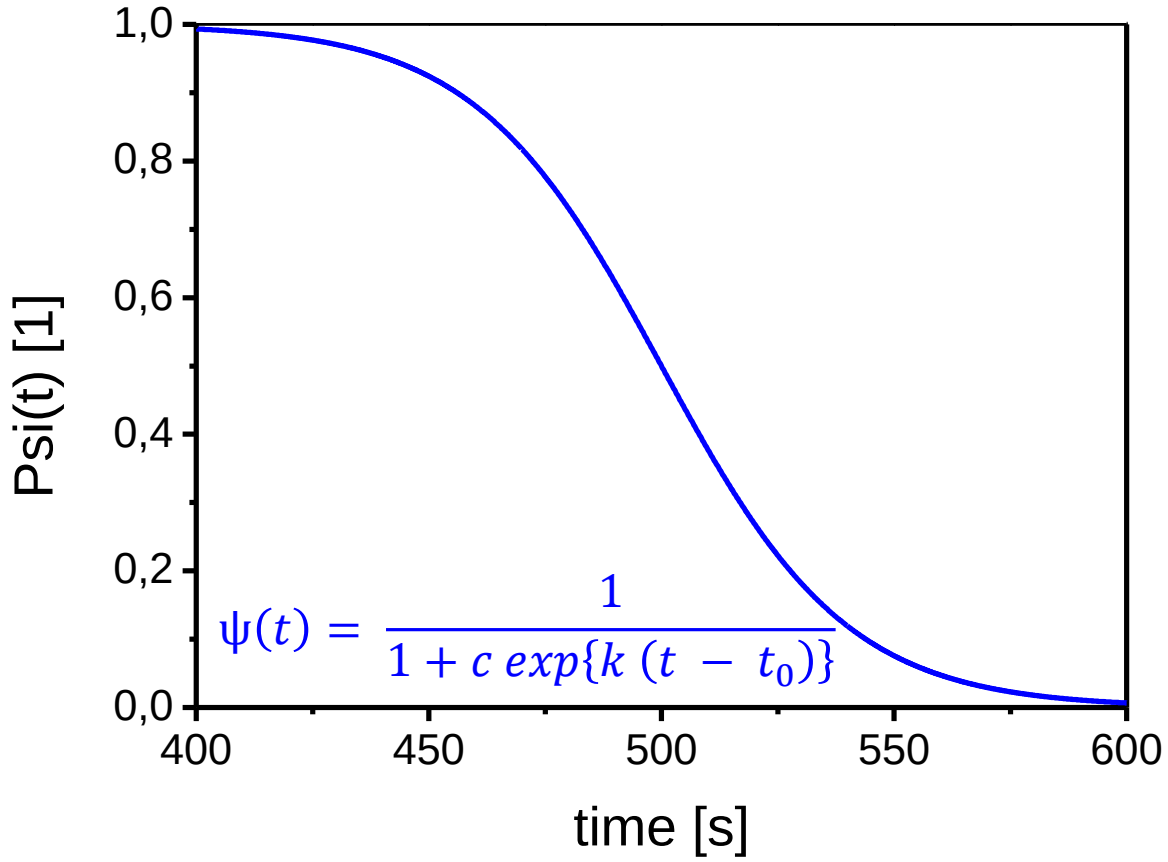
- Additional Assumptions
  - No side reactions
  - No or negligible diffusion of vanadium ions
- Applying FARADAY's law, the constant current leads to a constant change rate in the state-of-charge of the vanadium oxygen fuel cell
  ➔ the time variable can be replaced by a state-of-charge variable
- The inlet concentrations of the species are either a function of the state-of-charge (vanadium electrolyte half-cell) or constant (air half-cell)
- Taking all of this into consideration, the time-dependent simulation can be replaced by the stationary simulation with a state-of-charge parameter study

Performance degradation by flooding



Fraunhofer ICT

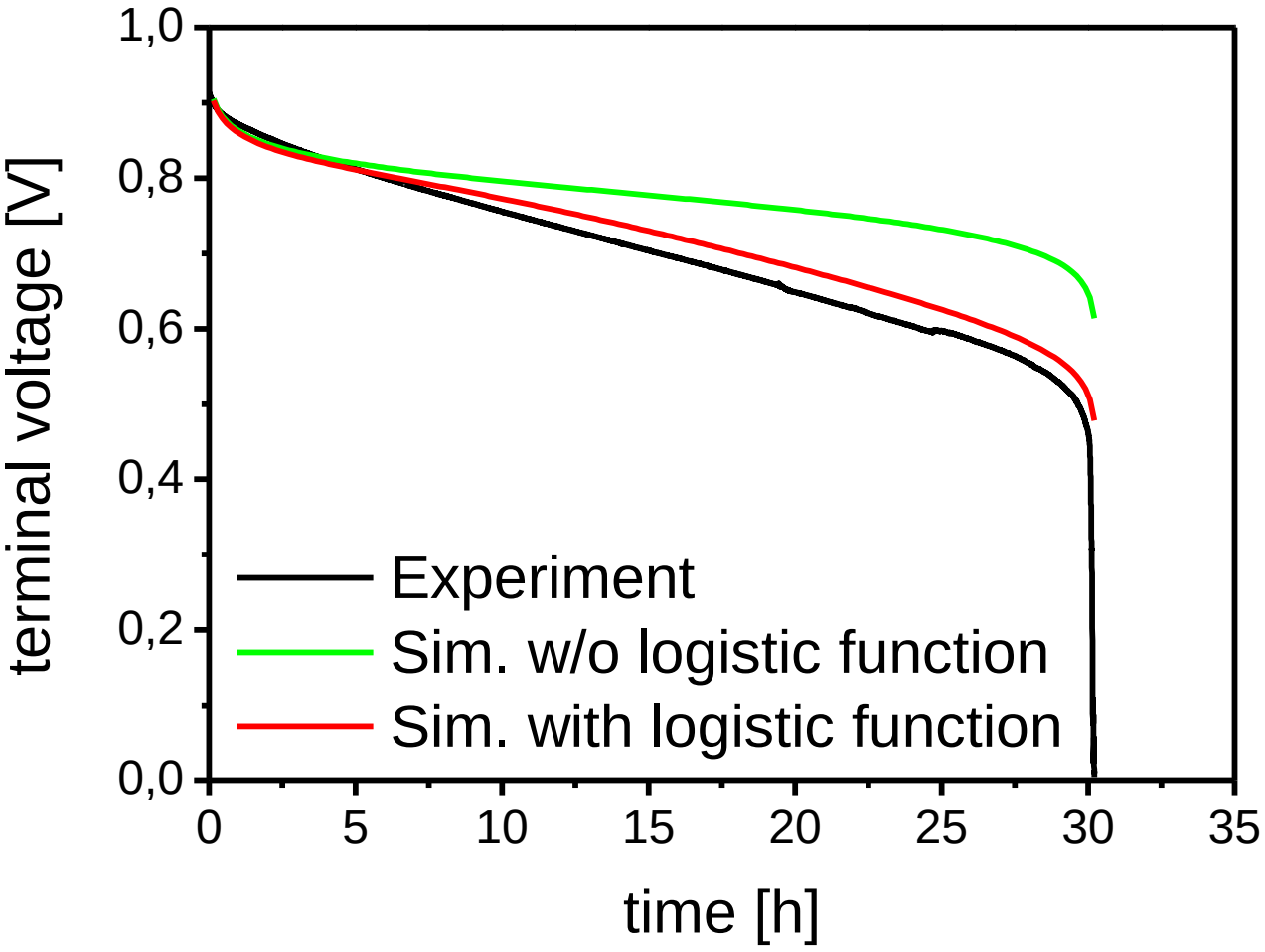
Expanding the stationary model (2)



$$j_{cath} = S_V\ \psi\ j^0_{cath}\ \frac{c^s(O_2)}{c^{ref}(O_2)} \left(-exp\left\{-\frac{\alpha_c\ \mathfrak{F}}{\mathfrak{R}\ T}\ \eta_c\right\}\right)$$

Fraunhofer ICT

Resulting Simulation



Fraunhofer ICT

Summary and outlook

- Vanadium Oxygen Fuel Cell as an interesting energy storage device
- Our design can be modeled and simulated using COMSOL Multiphysics
- Simulated data from stationary model shows very good agreement with experimental data
- Time-dependent simulation does not consider degradation process
- Altered stationary model can account for cathode degradation and reduce time-dependent simulation to a stationary parametric study of SOC, thus saving computing time

- Model enhancement
  - Thermal effects
  - Membrane cross-over effects

Thank you for your attention!

Dipl.-Ing. Frank Wandschneider
Fraunhofer-Institute for Chemical Technology
Department of Applied Electrochemistry
Joseph-von-Fraunhofer-Strasse 7
D-76327 Pfinztal / Germany
E-Mail: frank.wandschneider@ict.fraunhofer.de

COMSOL CONFERENCE ROTTERDAM2013

The authors gratefully acknowledge the funding by the Department of Commerce of the German Federal State of Baden-Württemberg

Ministerium für Finanzen und Wirtschaft Baden-Württemberg

Fraunhofer ICT