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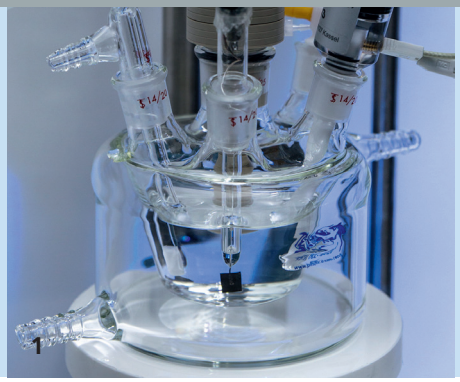

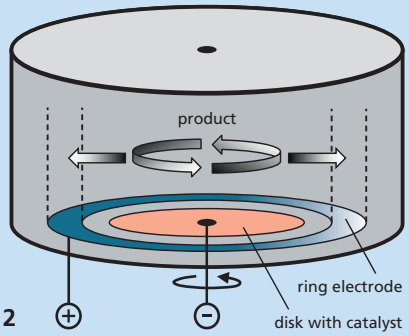

STROM
ALS ROHSTOFF

ROTATING RING-DISK ELECTRODE (RRDE) SIMULATION SOFTWARE

1 *Photograph of an RRDE measurement setup*

2 *Sketch of an RRDE measurement cell*

An RRDE simulation toolbox for catalyst evaluation

Rotating ring-disk electrode (RRDE) measurement cells are widely used experimental systems for electrochemical catalyst development and screening. The setup consists of a circular disk plated with catalyst material, and a concentric ring electrode (see fig. 1). The rotation of the electrodes induces a forced flow of the electrolyte, dragging solved reactants towards the disk. The flow transports the electrochemical product generated at the disk surface radially outwards to the ring electrode. At the ring, the product is reconverted and the resulting electrical ring current is detected to gain information about the catalyst quality and the reaction kinetics. In order to retrieve this information from the measured curves, a mathematical model is required.

We provide efficient simulation software for detailed analysis of RRDE measurements. Experimental data is read into the numerical toolbox, the generation of results happens fast and an automatic visualization of results is provided. This enables the experimenter to quickly and conveniently evaluate her or his data. The method can:

- handle arbitrary reaction mechanisms,
- distinguish reaction channels,
- calculate electro-kinetic parameters.

Particularly the first of the three points makes our method superior to existing analytical theories which are limited to special electrochemical reactions mechanisms.

We implement the method in any framework according to customer requirements, including a graphical user interface.

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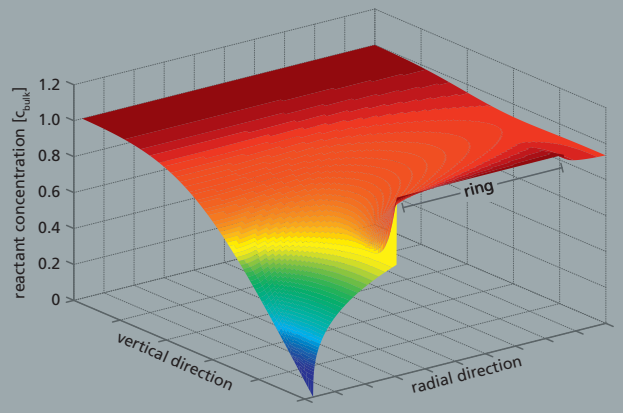

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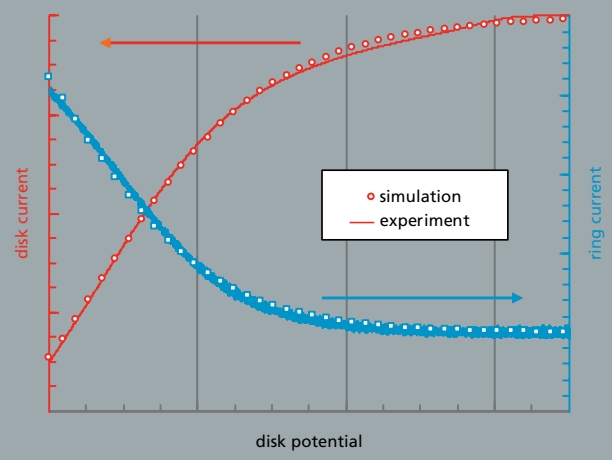

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3 *Calculated spatial concentration profile of a solved reactant normalized to its bulk concentration c_{bulk}*

4 *Measured disk and ring currents (lines) and the corresponding simulated points (markers) adapted to the measured curves by varying the electro-kinetic parameters*

Powerful simulation back-end

The numerical technique is based on a solution of a boundary value problem of the convection-diffusion equation (so far in MATLAB). The cylindrical symmetry of the system is exploited to restrict the calculations to two dimensions. The equations are discretized in a finite difference scheme with backward differences in order to utilize information from upstream. The Butler-Volmer model is employed to describe electrode kinetics, and the flow is included using an analytical series approximation which is known to yield results with an accuracy comparable to that of a rigorous numerical solution of the Navier-Stokes equations. However, since the flow equations are not solved here, the run-time of the simulations is heavily decreased. The outcome of the simulations consists in steady-state concentration profiles such as the one in fig. 2, from which the electrical currents at the disk and the ring electrode are calculated. The calculated currents are set into relation to the corresponding experimental values by taking their differences and minimizing a least-squares objective function in an outer optimization procedure. The algorithm iteratively adapts the simulation results to the measured currents (see fig. 3) by changing the electro-kinetic parameters of the underlying reaction mechanism. Reactant concentrations in the bulk or diffusion coefficients can also be determined in this manner. An article about the simulation technique and its application to the oxygen reduction reaction (ORR) mechanism at $PdAu_3$ surfaces was lately submitted to J. Electrochem. Soc.

(Martin von Kurnatowski: Quantitative kinetic analysis of a $PdAu_3$ alloy catalyst for oxygen electro-reduction, submitted to J. Electrochem. Soc., 2017).

Our Offer

- Implementation of an RRDE simulation software (e. g. for distribution with RRDE measurement cells) including a graphical user interface for experimenters to analyze their data rapidly and in detail
- Simulations on demand
- The software serves as a versatile platform for data selection and model fitting.
- Experimental tests for validation of the numerical software