Energy Transition
RESEARCH & INNOVATION

SÃO PAULO, BRAZIL | NOVEMBER 7-9, 2023

Energy Transition Research & Innovation Conference

ETRI 2023

BOOK OF ABSTRACTS

Research Centre for
Greenhouse Gas Innovation

USP

FAPESP

ETRI 2023 was sponsored by

Energy Transition Research & Innovation Conference

ETRI 2023

São Paulo, November 7-9, 2023

BOOK OF ABSTRACTS

ETRI Organization:
Karen Louise Mascarenhas – Conference Chair
Julio Romano Meneghini – Conference Co-Chair
Suani T. Coelho – Scientific Committee Chair
Alberto José Fossa – Scientific Committee Co-Chair

ETRI Logistics Secretariat:
Laura Emilse Brizuela
Vanessa Pecora Garcilasso
Silvia Cruso

RCGI Design & Communication:
Karen Louise Mascarenhas
Laura Emilse Brizuela
Silvia Cruso

We gratefully acknowledge the support of the RCGI – Research Centre for Greenhouse Gas Innovation (23.1.8493.1.9), hosted by the University of São Paulo (USP) and sponsored by FAPESP – São Paulo Research Foundation (2020/15230-5) and Shell Brasil, as well as the strategic importance of the support given by ANP (Brazil's National Oil, Natural Gas and Biofuels Agency) through the R&DI levy regulation.

DOI: 10.5281/zenodo.12744754

Preliminary conclusions: As mentioned earlier, the project has just started, and it has not been possible to obtain preliminary conclusions. The resulting analysis will be reported later.

Enrique Adalberto Paredes Salazar
University of São Paulo

Abstract Title: Understanding Electrocatalytic Reactions trough Microkinetic Modelling Approaches

Authors' Names & Affiliation Institutions of all authors (in order for publication):
São Carlos Institute of Chemistry - University of São Paulo
GIFBA - Universidad de Nariño
São Carlos Institute of Chemistry - University of São Paulo

Abstract: A profound comprehension of the intricate interplay between reactive and intermediate molecules and the electrode surface at the microscopic level is essential for advancing our understanding of (electro)catalysis. These interactions have profound implications for the overall catalytic activity of materials, operating at the mesoscopic level. In this sense, microkinetic modelling is a powerful approach that bridges these two levels by unravelling the global kinetics of a reaction from the contribution of each individual step within the reaction mechanism. Here, we present a systematic methodology for constructing a robust microkinetic model, encompassing four crucial stages: (i) gathering information and mechanism statement, (ii) model establishment, (iii) numerical simulations,
and (iv) comparison with experiments. To demonstrate the efficacy of this methodology, we applied it to investigate the mechanisms governing the electrooxidation reactions of formic acid and methanol. In the final stage of the methodology, experiments under oscillatory dynamics proved to be a remarkably sensitive tool for model validation. Compared to traditional techniques such as cyclic voltammetry (CV) and chronoamperometry (CA), these experiments exhibited superior sensitivity to changes in the reaction mechanism and rate constants for each elementary step. Furthermore, we conducted a sensitivity analysis on our models, quantifying

the individual contributions of each reaction step within the electrocatalytic system towards the overall oscillatory response. This comprehensive approach not only enhances our understanding of (electro)catalytic processes at the microscopic level but also paves the way for the development of materials with greatly improved catalytic properties.

Keywords: Methanol electro-oxidation, formic acid electro-oxidation, microkinetic modelling, oscillations, numerical simulations.

Introduction and Objectives: A thorough understanding of the intricate interplay between reactive and intermediate molecules and the electrode surface at the microscopic level is essential for advancing our understanding of (electro)catalysis. These interactions have profound implications for the overall catalytic activity of materials, operating at the mesoscopic level. In this context, microkinetic modelling emerges as a powerful approach, bridging the gap between these two levels by unravelling the global kinetics of a reaction through a meticulous examination of each individual step within the reaction mechanism. Here, our goal is to introduce a systematic methodology for building a robust microkinetic model.

Methodology: The construction of a microkinetic model encompassing four crucial stages:

(i) gathering information and mechanism statement,
(ii) model establishment,
(iii) numerical simulations,
(iv) validation through experimental comparisons.

To demonstrate the efficacy of this methodology, we applied it to investigate the mechanisms governing the electrooxidation reactions of formic acid and methanol.

Preliminary results: Experiments under oscillatory regime proved to be more sensitive for model validation compared to traditional techniques such as cyclic voltammetry (CV) and chronoamperometry (CA), as they showed superior sensitivity to changes in the reaction mechanism and rate constants for each elementary step.

Preliminary conclusions: This approach improves our understanding of (electro)catalytic processes at the microscopic level by evaluating the kinetic response at the mesoscopic level, paving the way for the development of materials with greatly improved catalytic properties.

Fátima Eduarda do Nascimento Morais
USP

We gratefully acknowledge the support of the RCGI – Research Centre for Greenhouse Gas Innovation (23.1.8493.1.9), hosted by the University of São Paulo (USP), sponsored by FAPESP – São Paulo Research Foundation (2020/15230-5), and sponsored by TotalEnergies, and the strategic importance of the support given by ANP (Brazil's National Oil, Natural Gas and Biofuels Agency) through the R&DI levy regulation.