TKTD models for aquatic primary producers – a new SETAC working group
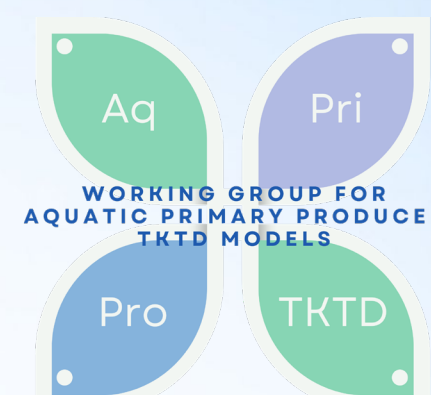
Hommen U[1], Mangold-Doering A[2], Reichenberger S[3], Witt J[4], Rendal C[5]

[1]Fraunhofer IME, [2]WUR, [3]knoell France SAS, [4]Bayer, [5]Syngenta

Who are we?

Working Group (WG) — a vibrant community of 20+ experts coming together monthly since Autumn 2024

Our members bring expertise in **modelling**, **biology**, and **risk assessment**, with a well-balanced mix from both **academia & industry**

Still missing a key piece of the puzzle: **regulatory representation** — we welcome collaboration!
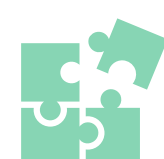
We need you!

Meet us at the Open Meeting of the SETAC Europe Interest Group on Effect Modelling (SEIGEM) on Monday May 12th from 4-5 pm in room 0.14!

Contact Us!

cecilie.rendal@syngenta.com
annika.mangold-doering@wur.nl

Activities until now

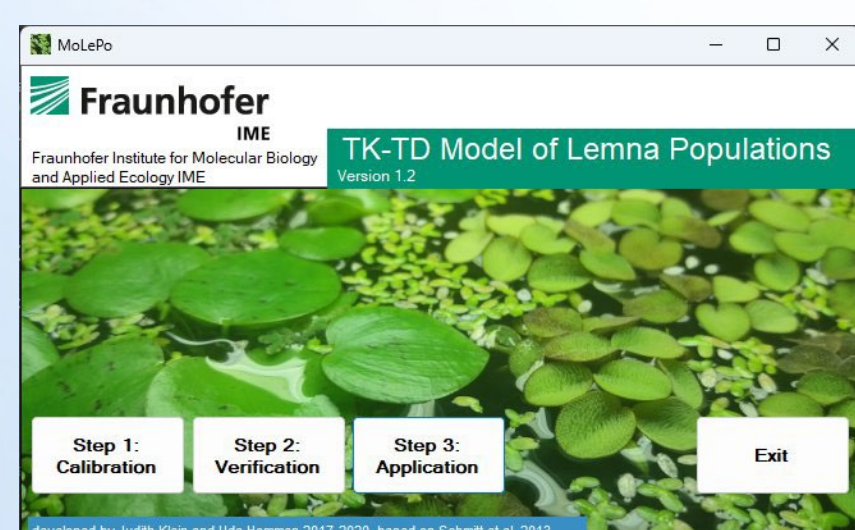Introduction of available software:
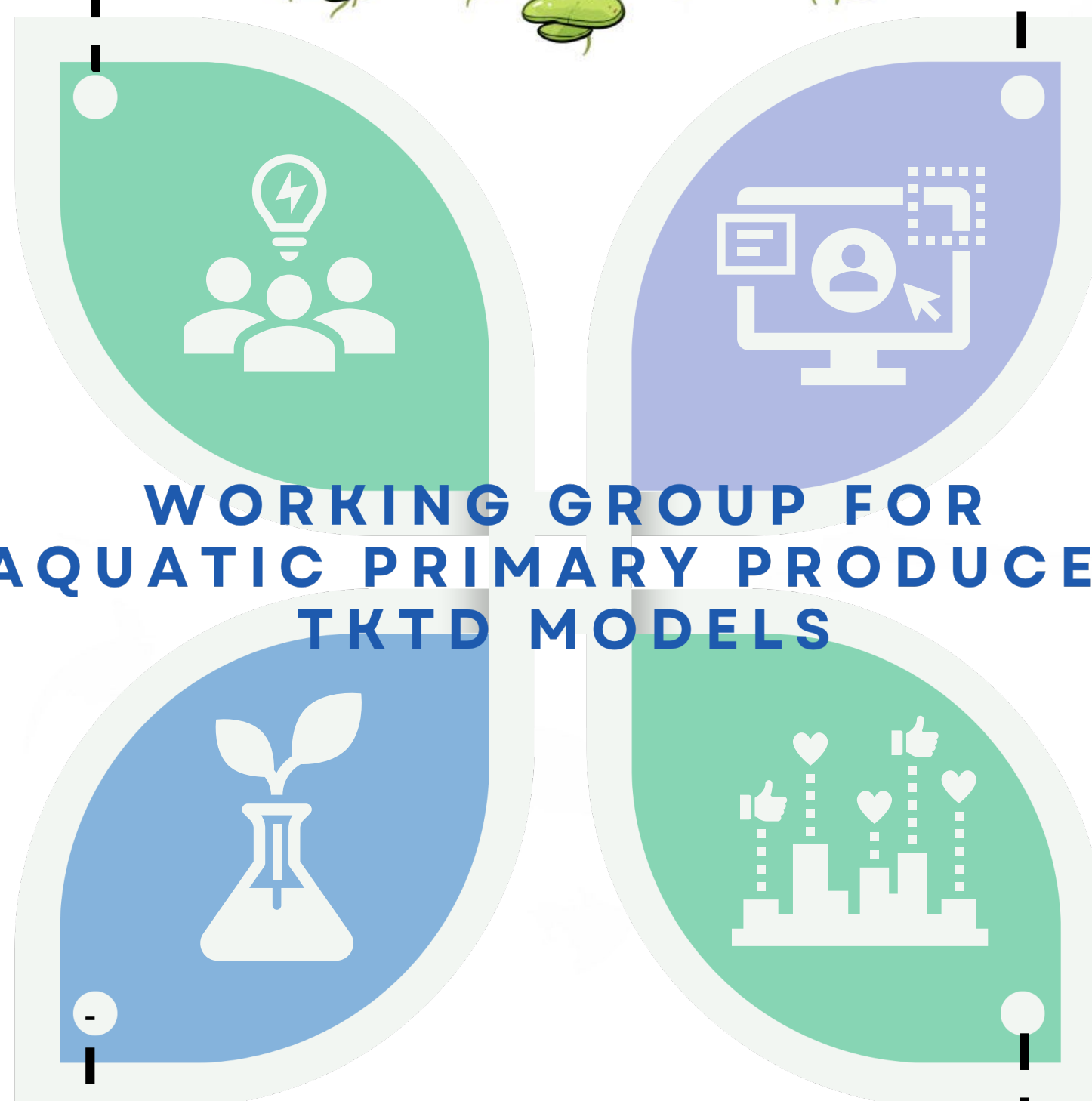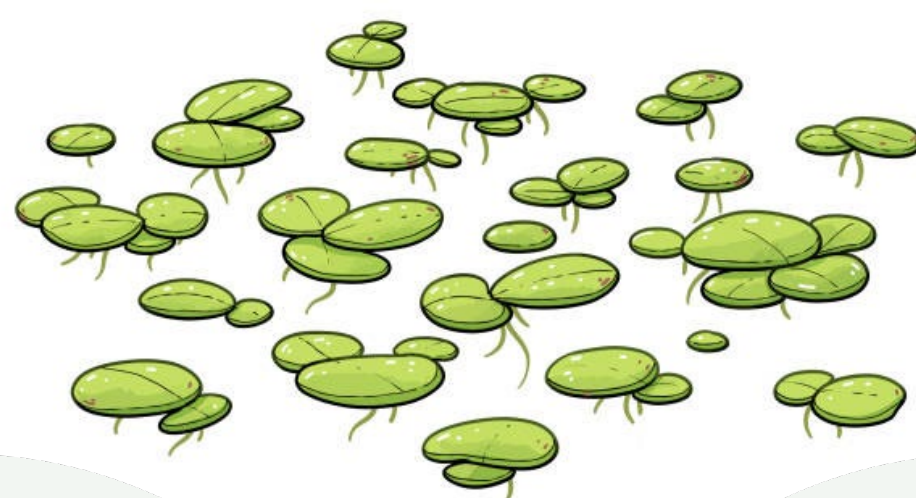- **cvasi – R package** [1] presented by Johannes Witt

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cvasi: Calibration, Validation, and Simulation of TKTD models in R

CRAN 1.4.0 R-CMD-check passing

The `cvasi` package aims to ease the use of ecotox effect models by providing an intuitive workflow. Model inputs and parameters are encapsulated in scenario objects which can be piped to other functions. Operations can be chained using the `tidy` syntax. The most time-consuming processes can be run in parallel if requested.

- **MoLePo – Software** [2] presented by Judith Klein

Fraunhofer IME
Fraunhofer Institute for Molecular Biology and Applied Ecology IME
TK-TD Model of Lemna Populations
Version 1.2

Step 1: Calibration Step 2: Verification Step 3: Application Exit

Developed by Judith Klein and Udo Hommen 2017-2024, based on Schmitt et al. 2013

WORKING GROUP FOR AQUATIC PRIMARY PRODUCER TKTD MODELS

Discussions on the **Checklist for Primary Producer Models** in **EFSA PPR (2018)** [1] by Cecilie Rendal & others

Checking ANNEX C for:

✓ Applicability of current list
✓ Updates needed in light of new studies
✓ Identify potential gaps & develop solutions

Discussion on topics in macrophyte risk assessment:
- Presentation on **sensitivity analysis** by Stefan Reichenberger
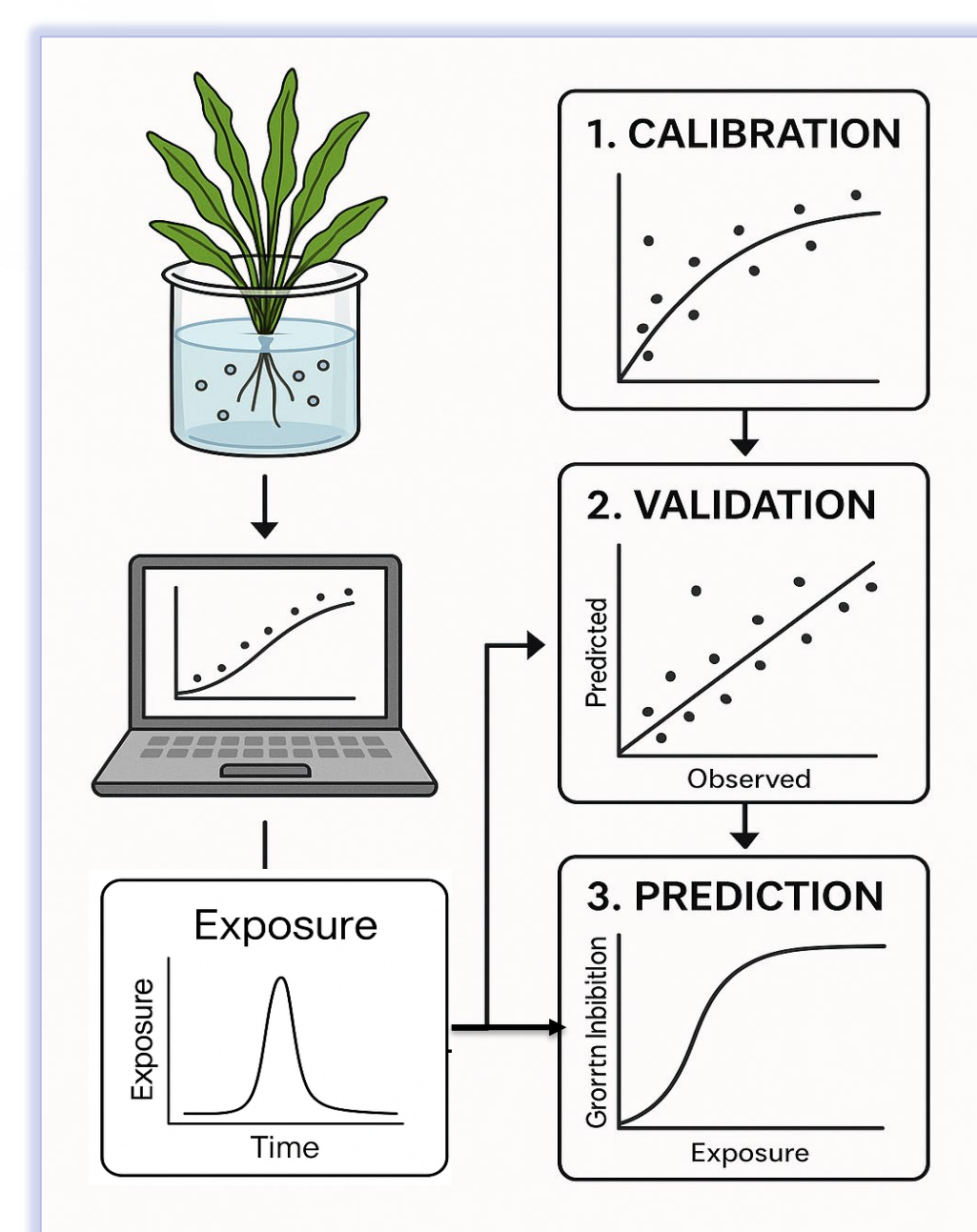- Presentation **on growth rates** by Johannes Witt

Our Objectives

Develop a **unified strategy** for **calibration** and **validation** of TKTD models for aquatic primary producers

Support **Tier 2C** assessments, **predicting effects** under dynamic FOCUS exposure profiles

Create and test **user-friendly, open-source software** to support practical application

1. CALIBRATION
2. VALIDATION — Predicted / Observed
3. PREDICTION — Growth inhibition / Exposure
Exposure / Time

Envisioned Output

Presentations at SETAC meetings

Report available on the SETAC website

A publication, e.g., **short communication**

References:
[1] Kehrein N, Nickisch D, Vermeiren P (2025). cvasi: Calibration, Validation, and Simulation of TKTD Models. https://doi.org/10.32614/CRAN.package.cvasi
[2] Klein, J, Hommen, U (2018). TK-TD model of Lemna populations (MoLePo). https://www.ime.fraunhofer.de/en/Research_Divisions/Division_AE/Software_E/MoLePo.html
[3] EFSA PPR Panel (2018). Scientific Opinion on the state of the art of Toxicokinetic/Toxicodynamic (TKTD) effect models for regulatory risk assessment of pesticides for aquatic organisms. https://doi.org/10.2903/j.efsa.2018.5377