

The Persistence Assessment Tool (PAT): implementing a methodology for data quality evaluation and weight of evidence in persistence assessments



Chris Hughes¹, Megan Griffiths¹, Simon Cook¹, Dik van de Meent², John Parsons², Delina Lyon³, Amelie Ott⁴

¹: Ricardo Energy & Environment, Harwell, UK | ²: Association of Retired Environmental Scientists (ARES), Odijk, NL | ³: Concawe, Brussels, BE | ⁴: ICCS, New York, USA.

Email contact:
chris.hughes@ricardo.com

INTRODUCTION

- Regulatory persistence assessment involves comparing degradation half-lives to criteria in environmental compartments. Other information is also relevant (e.g. biodegradation screening tests, non-standard experiments, quantitative structure activity relationships (QSARs), field data, etc), and should be considered following a weight of evidence (WoE) determination.
- However, there are challenges relating to evaluating the quality (reliability and relevance) of persistence data, and in applying this in a robust, transparent and consistent WoE determination. There are also issues for substance types that are challenging to evaluate using standard methods.
- To address these challenges, a software tool – the Persistence Assessment Tool (PAT) – has been developed to support the evaluation of persistence.
- The tool provides a step-by-step process that systematically captures, evaluates and combines degradation data to assess persistence in line with global regulatory frameworks.
- Methodologies have been developed to 1) score the quality of diverse degradation data, 2) evaluate lines of evidence (LoE), and 3) conduct a quantitative WoE determination to calculate a persistence conclusion.
- A multimedia fate model is also included to calculate overall persistence (P_{ov}).

AIM: To implement a methodology for the systematic evaluation of data quality and weight of evidence determination, providing support to practitioners for the robust, consistent and transparent assessment of persistence under different regulatory frameworks.

METHODOLOGY

1 Data quality scoring

- Rules have been developed to evaluate the quality of individual studies.
- Scores are produced for **individual fields** > **categories of fields** (e.g. test system, inoculum, kinetics) > **reliability/relevance** > and **overall quality**.
- Identified **difficult substances** have certain **flags** and considerations during scoring, such as testing volatile substances in an open system.
- Fields are scored as 0, 5 or 10 according to individual quality criteria. Some fields have potential '**critical fails**', which lead to a score of 0 for either reliability and/or relevance, such as evidence of using a pre-adapted inoculum.
- Each study is scored by sequential averaging of scores:



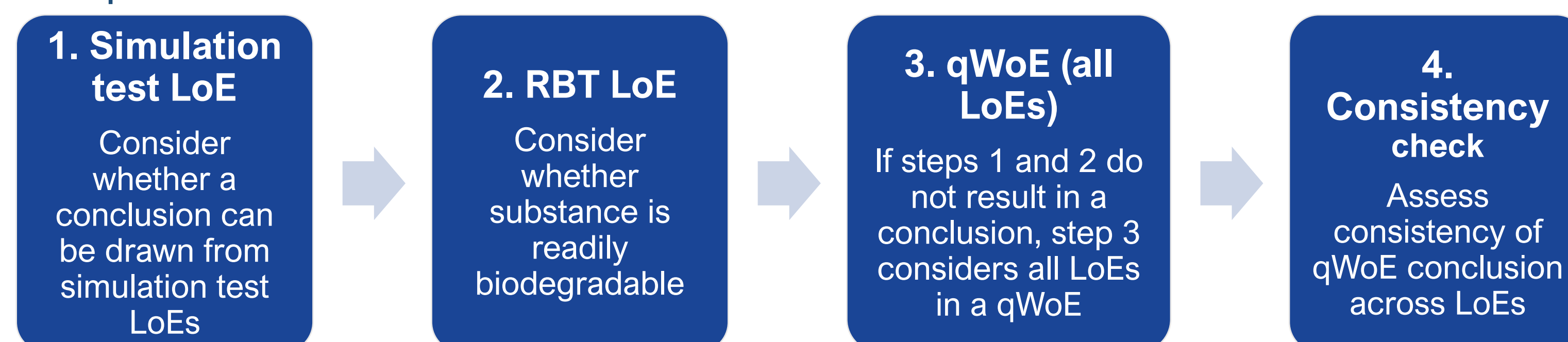
- Numerical scores are rated qualitatively as low (L, 0 to <4), medium (M, 4 to <7), or high (H, 7 to 10).

2 Line of Evidence (LoE) evaluation

- Each study is combined with other studies from the same line of evidence (LoE) to reach conclusions at the LoE level.
- The LoEs are: simulation tests for water, sediment and soil, screening tests, QSARs, monitoring data, and other relevant data ('other WoE').
- The evaluation includes an assessment of the **persistence outcome** and the **strength of the evidence** for each LoE.
- Depending on the LoE, strength of evidence may incorporate **quantity** (how many useable data), **quality** (whether the data are M or H), **magnitude** (by how much is the P/vP criterion exceeded), and **consistency** (how much of the LoE dataset agrees with the conclusion).
- A representative half-life is produced for the simulation test data, temperature-corrected by default to 12°C for soil and fresh/estuarine water and sediment, or 9°C for marine water and sediment. The determination of the representative half-life for the LoE depends on the number of suitable (M or H quality) data available.

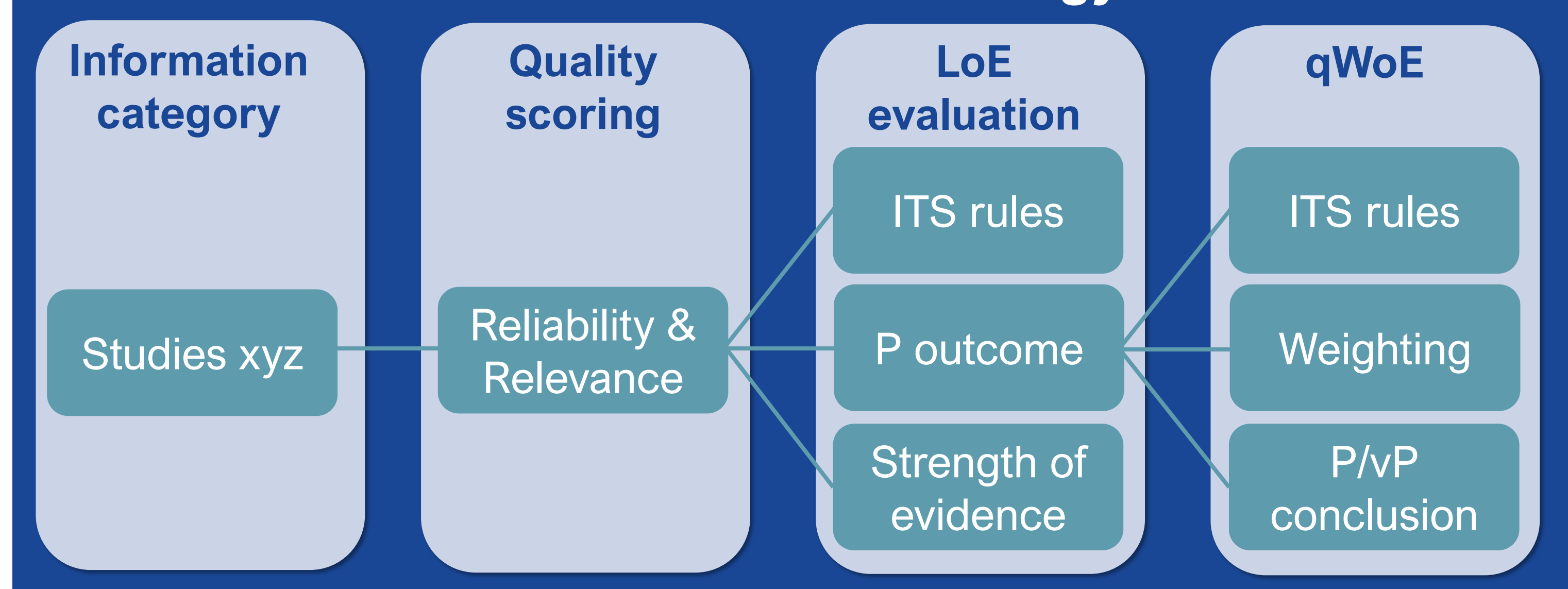
3 Quantitative Weight of Evidence (qWoE)

- The overall conclusion of the persistence assessment is reached following a step-wise scheme:



- The workflow prioritises the **simulation test LoE** (Step 1) as these generate definitive half-lives for comparison to P/vP criteria, followed by the **ready biodegradability test (RBT) LoE** (Step 2), as per the EU REACH integrated testing and assessment strategy (ITS). Steps 1 or 2 can be switched off.
- If a conclusive outcome cannot be reached from Step 1 or 2, a **qWoE methodology** is applied considering all LoEs together (Step 3).
- The qWoE methodology applies a scoring system to each LoE that considers the persistence conclusion, strength and LoE weighting.
- The overall score for each LoE determines its persistence indication; a positive score indicates 'persistent' while a negative score indicates 'not persistent', and the size of the score indicates strength of indication.
- The overall scores of each LoE are then averaged to determine a mean score and subsequent overall conclusion for the persistence assessment.
- A **consistency check** (Step 4) is also performed to determine how many LoEs align with each persistence outcome.
- The multimedia fate model SimpleRisk4PAT (based on SimpleBox) has been integrated to calculate P_{ov} using representative half-lives from PAT.

Overview of Methodology



CONCLUSIONS

- The PAT methodology enables a systematic evaluation of data quality and WoE determination of persistence under EU REACH and other regulatory frameworks.
- There is a need for stakeholder input to support further validation, consensus-building and uptake of the methodology.

Scan to download, join the user community and register for our free training webinar!

