PetroRisk version 8.01: Improved model for performing REACH environmental risk assessments on petroleum substances

This article provides an overview of the improved PetroRisk model, which was released on 27 July.

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The REACH Regulation requires registrants to perform an environmental risk assessment (ERA) on each hazardous substance manufactured or imported above a total annual EU tonnage of 10 tonnes. An ERA compares the estimated concentration of the substance in the environment (based on its volume and emissions) with the toxicity of the substance; if the concentration in the environment exceeds the concentration at which it becomes toxic, then the registration is disallowed.[1]

Due to their UVCB[1] nature, petroleum substances (PS) necessitate a complex and tailored ERA approach: PS contain an indeterminably large and variable number of different hydrocarbon constituents, which all partition, degrade and exert toxicity differently once released to the environment. Initially, the ERA requires (a prediction of) the identity and concentrations of the constituents released to the environment (to air, water and soil) during each use of the PS. Subsequently, the fate of each emitted constituent in the environment is modelled separately, based on predicted constituent properties and 'generic' environmental conditions. Finally, the predicted concentrations in the different environmental compartments (such as marine sediment, or terrestrial worms) are compared to compartment- and constituent-specific toxicity thresholds (the predicted no-effect concentration), in the form of a 'risk characterisation ratio' (RCR, see equation below). Due to the additive nature of hydrocarbon toxicity (narcosis), the compartment-specific RCRs of the *n* constituents can be summed up to compartment-specific RCRs representing the entire PS:

$$\textit{Risk characterisation ratio (RCR)} = \sum_{i=1}^{n} \frac{\textit{Predicted environmental concentration (PEC)}_i}{\textit{Predicted no-effect concentration (PNEC)}_i}$$

If all compartment-specific RCRs are equal to, or lower than, a value of 1, the risks for adverse environmental effects resulting from the use of the substance are considered adequately managed, and the use can be considered 'safe'. If one or more RCRs have a value above 1, then risk management measures need to be applied to reduce the emissions from use to 'safe' levels.

[1] Chemical substances of unknown or variable composition, complex reaction products and biological materials

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To enable the execution of the ERAs for its 2010 product registrations, Concawe commissioned an Excel™-based tool, called PetroRisk. Major innovations compared to existing ERA tools include the following:

- The use of the so-called 'hydrocarbon block method', which extrapolates analytical data of a PS (for example two-dimensional gas chromatography (GCxGC)) to representative concentrations of hydrocarbon constituents.
- The use of a 'constituent library', which contains the required (predicted) physicochemical and degradation properties for 1,560 representative constituents.
- The use of a 'fate-factor' (FF) library. Each FF linearly extrapolates a specific emission (e.g. waste water) of a specific constituent (e.g. naphthalene) to the predicted concentration in a specific environmental compartment (e.g. marine sediment). The FF approach allows the user to 'shortcut' many calculations which are independent of PS composition, use conditions and emission levels.

For other stakeholders to benefit from PetroRisk, the model was made freely available on Concawe's website.

Since 2017, an increasing number of improvements to PetroRisk have been identified by the Concawe Secretariat, culminating in a complete reorganisation and optimisation of the model using a more transparent interface during 2021–2022.

Major innovations in the updated model are described below:

- A visual representation of the data flow (see Figure 1 on page 30), and the possibility to review the data after each calculation step.
- Full alignment of the basic ('Tier 1') model with the ECHA Guidance.
- Update of the embedded fate models (sewage treatment plant, regional environment and human exposure) and implementation of hydrocarbon-specific parameters.
- The application of a minimalistic FF concept, covering only the complex and extensive calculations of the fate in a sewage treatment plant and in the regional environment. All other calculations embedded in the previous FF concept have now been implemented as individual calculations in PetroRisk, thereby increasing the transparency and flexibility of the model.
- Robust calculation and facultative implementation of a minimal set of air and wastewater RMM[2] efficiencies required to achieve safe emission levels.
- Implementation of a batch mode, allowing the tool to consecutively execute ERAs for many substances. While previously two working weeks were required, the updated model requires about three hours to perform ERAs on all Concawe substances.

[2] Risk Management Measures

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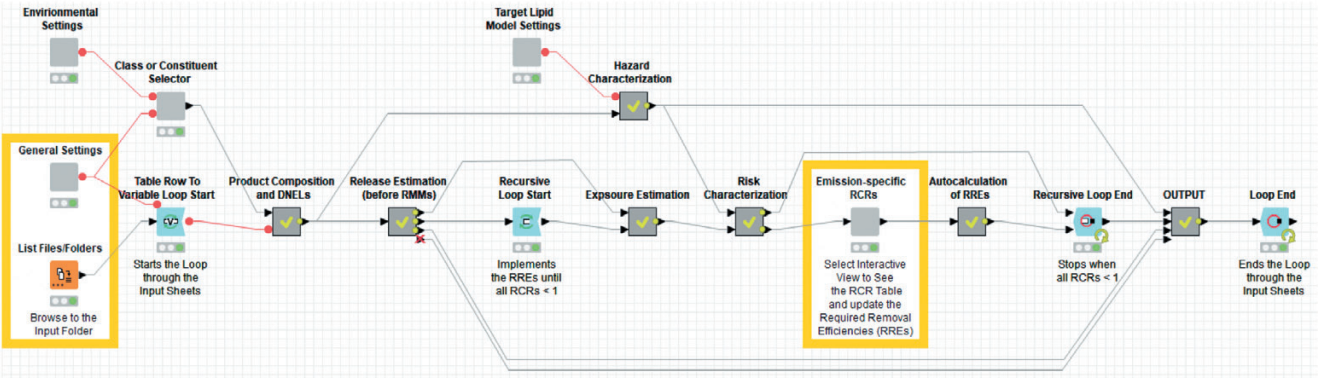
Figure 1: The KNIME PetroRisk v8.01 workflow



PetroRisk has been programmed as a workflow in the Konstanz Information Miner (KNIME), which is an open source data analytics, reporting and integration platform based on Eclipse and written in Java. An intuitive drag and drop style graphical user interface allows visual assembly, execution and analysis of complex workflows without the extensive need for programming skills.

The updates result in a model which is (1) faster, (2) more transparent, (3) better aligned with ECHA Guidance, (4) more applicable to hydrocarbons and (5) more user-friendly. Compared to previous PetroRisk versions, version 8.01 generally predicts lower risks for professional and consumer uses, but higher risks for industrial uses.

PetroRisk version 8.01 was released on 27 July and is available free-of-charge from the Concawe website.[3] There have already been two Concawe training sessions on the general REACH ERA concept[4] and on the PetroRisk tool.[5] The tool will be accompanied by a detailed manual and a dedicated scaling tool. The scaling tool is a simple Excel™ workbook designed to aid registrants and downstream users in assessing whether their specific use conditions are covered by a generic exposure scenario generated with PetroRisk.

Reference

1. ECHA (2016). *Guidance on information requirements and Chemical Safety Assessment. Chapter R.16: Environmental exposure assessment.* Version 3. https://echa.europa.eu/documents/10162/17224/information_requirements_r16_en.pdf/b9f0f406-ff5f-4315-908e-e5f83115d6af?t=1455553705739

[3] https://www.concawe.eu/reach/petrorisk

[4] https://youtu.be/Icg3ANNiz2M

[5] https://youtu.be/nnP5tOtMSm8