



New software development for automated environmental fate modeling and reporting by Dr. Knoell Consult GmbH

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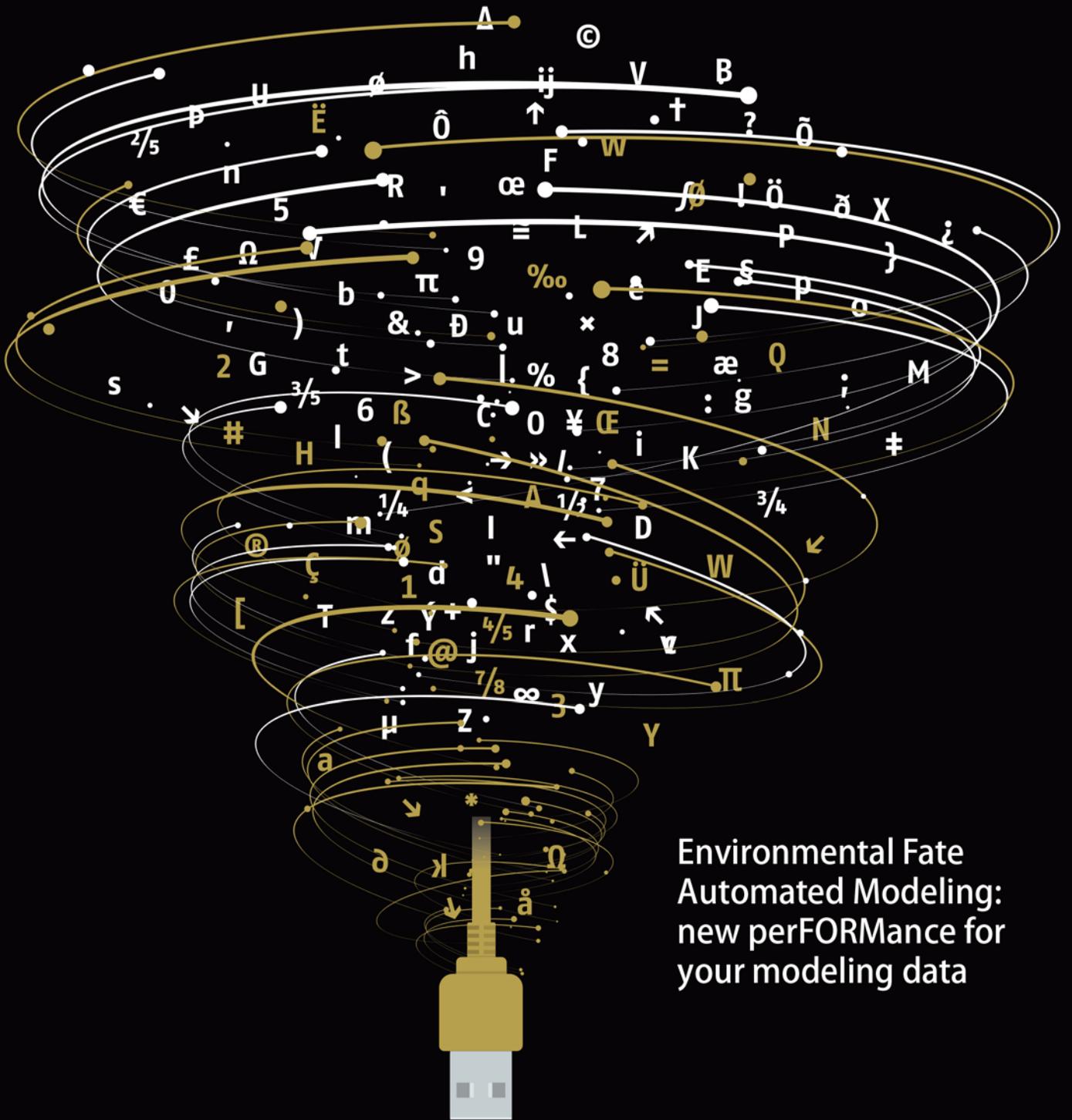
Abstract

With the newly developed software product we will offer a web-based application for automating environmental exposure assessments prescribed for approval procedures for plant protection products (PPP). Such exposure assessments are performed using established computer models. The software will be able to automate and optimize the workflow for individuals or groups of people dealing with environmental fate and exposure assessment. It is developed to automate model parameterization and model simulations, extract the results and transfer the output to formatted tables suitable for dossier/report incorporation. The development is of interest, not only in terms of speeding up modeling and report generation, but also it will optimize the organization of data, reduce the occurrence of manual input errors and reduce the effort required for quality control.

For the registration of plant protection products the agrochemical industry needs to provide environmental risk assessments for active substances and related products. To conduct these risk assessments, obligatory and officially provided third-party computer models are used in many countries worldwide. Scenarios and model parametrization are described in publicly accessible guidance documents. The computer models are used to obtain an estimate of the amount of substance that will enter the environment (Predicted Environmental Concentrations, PEC). PECs are calculated for different environmental compartments by different simulation models.

To minimize the influence of the user on the outcome of the PEC estimation, in process oriented regulatory models as many as possible of the input variables have been fixed and were aggregated to different scenarios, leaving only the substance-specific dossier data as main inputs. To take care of this input process and to guide the user through the correct scenarios to run depending on the use of the PPP, a graphical user interface is provided for all relevant models. This shell helps the user through the exposure assessment. However, each model that is used in the registration process needs to be parametrized individually. Hence, in an environmental risk assessment several different models need to be set-up, parametrized, or run separately. This decentralized working procedure unfortunately implies significant drawbacks. The main disadvantages are: replicated entry of identical input data, great extent of manual work, high quality assurance effort, challenging data management due to scattered information of the input/output files, and time-consuming workflow documentation. Furthermore, there is a need for optimization of the overall modeling workflow in order to efficiently manage the ever-increasing complexity of the registration process itself (data requirements, national-specific modeling approaches etc.), but also the strict submission deadlines set by the authorities.

As a consequence, Dr. Knoell Consult GmbH started to develop a software package to facilitate automated environmental exposure modeling and reporting. The aim was to create a software application that can drive all necessary computer models and evaluate the results from one single platform in an automated manner. The software is developed in a modular structure



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allowing for individual integration of modeling tools. This structure enables flexible adaptation at the modular-level, e.g. when new regulatory models are released, or new model versions are made available and need to be applied. The software suite will be provided as a web-based solution accessible through a common web browser. Model calculations will no longer need to be carried out on desktop computers, but will be performed on a more powerful and remote server located in a secured data center, constantly maintained by our internal information technology department. These features minimize the computational burden on the end-user's personal machine. The modeling workflow within organizations is bundled and the overall exposure assessment is organized into modules available via a single project.

The centralized and automated way in which the environmental modeling and risk assessment will be performed with the software offers many advantages compared to the common procedure. Input data used for modeling can be stored in one central database, reducing potential implementation of errors and quality assurance related issues often caused by significant amount of manual work. Workflow can therefore be organized in a more efficient and structured way. Due to its automated nature, the software will speed up environmental exposure modeling and

report generation. The implemented customizable reporting module will be able to automatically generate result tables directly suitable for the integration into submission dossiers or scientific reports. In general, the software can be seen as a tool to optimize the overall modeling and reporting performance in the registration process by reducing the time needed for parametrization and documentation.

At a glance

The software currently being developed by Dr. Knoell Consult GmbH automates running the exposure models, which are required by the approval process for plant protection products globally. These exposure assessments are accomplished with regulatory computer models, which are not developed by Dr. Knoell Consult GmbH. The software will be able to harmonize the parameterization of these models, starts them automatically, automatically extract the results and transfers them automatically to Excel and Word documents. The software will be located on Dr. Knoell Consult GmbH servers in a data center in Germany. The environmental fate automated modeling tool will continuously being updated and extended to reflect potential new models or new model versions. The tool will be offered to clients upon completion.



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