efam – New software development for automated environmental fate modelling and reporting

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Abstract
With the newly developed software product we present 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 optimise the workflow for individuals or groups of people dealing with environmental fate and exposure assessment. It is developed to automate model parametrisation 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 modelling and report generation, but also it will optimise the organisation of data, reduce the occurrence of manual input errors and reduce the effort required for quality control.

Background
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. 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. Hence, in an environmental risk assessment several different models need to be set-up, parametrised, or run separately. This decentralised 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. As a consequence, we started to develop a software package to facilitate automated environmental fate modelling and reporting.

Goal and Scope
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 allowing for individual integration of modelling 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.

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Characteristics
- Flexible modular structure
- Individual integration of modelling tools possible
- Adaptation at modular–level enabled
- Accessible through common web browser
- Calculations can be run on more powerful remote server instead of using desktop PC
- Significant runtime reduction through automated parallelisation of model runs

Advantages
- Faster handling of your modelling tasks
- Higher quality due to less amount of manual work
- Concentrate on your projects – not on tool development
- Safe use within knoell secured IT infrastructure
- Integration of any further model possible
- Basis for spatial explicit higher tier modelling

efam can help
- Centralise input data for several models in one database
- Reduce implementation errors often caused by manual work
- Optimise quality assurance procedures
- Speed up exposure modelling and report generation
- Automatically generate result tables suitable for submission dossiers and scientific reports
- Reduce time needed for model parametrisation and documentation