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Modelling exposure of workers, residents and bystanders to vapour of plant protection products after application to crops



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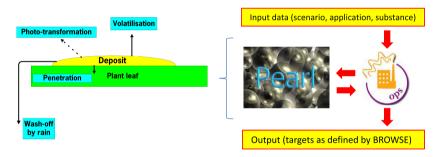
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HIGHLIGHTS

- A pesticide volatilisation model has been coupled to a dispersion model.
- The combined PEARL-OPS model has been tested against experimental data.
- A first conservative tier to assess vapour exposure has been developed.
- The sensitivity of the PEARL-OPS model to relevant input parameters is shown.
- Proposals are presented for higher tier options for vapour exposure assessments.

GRAPHICAL ABSTRACT

Modelling volatilisation (PEARL) and dispersion in air (OPS)



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$A\ B\ S\ T\ R\ A\ C\ T$

Agricultural use of plant protection products can result in exposure of bystanders, residents, operators and workers. Within the European Union (EU) FP7 project BROWSE, a tool based on a set of models and scenarios has been developed, aiming to assess the risk of exposure of humans to these products. In the present version of the tool only a first conservative tier is available for outdoor vapour exposure assessment.

In the vapour exposure evaluation, the target concentrations in air at 10 m distance from the edge of a treated field are calculated for specific scenarios for each EU regulatory zone. These scenarios have been selected to represent reasonable worst case volatilisation conditions. The exposure assessment is based on a series of weekly applications in a five year period to cover a wide range of meteorological conditions. The volatilisation from the crop is calculated using the PEARL model and this PEARL output provides the emission strength used as input for the short term version of the atmospheric transport model OPS.

The combined PEARL-OPS model is tested against measurements from a field experiment. First results of this test show that the mean concentration level was predicted fairly well. However, sometimes the differences between observations and simulations were found to be substantial. Improvements are suggested for the vapour exposure scenarios as well as for further model development.

In the current version of the BROWSE tool a simplified procedure is used to assess single and multiple applications. The actual period of application and the time of application during the day are fixed, and the growth stage of the crop cannot be taken into account. Moreover, competing processes such as penetration of the substance into the plant tissue are not considered. The effect of these factors on the target exposure concentrations is discussed.

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1. Introduction

Agricultural use of plant protection products can result in exposure of bystanders, residents, operators and workers. For registration of plant protection products within the European Union (EU), the risk must be assessed according to the new regulation 1107/2009. This regulation aims to protect humans and the environment against adverse effects of the agricultural use of plant protection products. Within the EU FP7 project BROWSE (Bystanders, Residents, Operators and WorkerS Exposure models for plant protection products) a tool based on a set of models and scenarios has been developed, in order to assess the risk of exposure of humans to these products. One of the components of this assessment is the vapour exposure for worker, resident and bystander. The BROWSE model of vapour exposure is based on two existing models, PEARL (Pesticide Emission Assessment at Regional and Local scales) and OPS (Operational Atmospheric Transport Model for Priority Substances).

In previous research on volatilization and dispersion of plant protection products, Raupach et al. (2001) applied a 3D Gaussian dispersion model approach, but used a relatively simple empirical model to describe source strength. Asman et al. (2003) combined a 2D dispersion model with an empirical volatilisation model. Jacobs et al. (2007) also used PEARL to describe volatilization, but in combination with a 2D version of OPS. Butler Ellis et al. (2010b) used an empirical volatilization model, but coupled it to an advanced atmospheric dispersion model (Atmospheric Dispersion Modelling System, ADMS). Bedos et al. (2013) coupled the mechanistic model Volt'air for bare soil volatilization to a 2D atmospheric dispersion model.

The model combination applied in the BROWSE tool computes 3D concentration patterns at short distance around treated fields, using PEARL as the volatilization (source strength) model and a special 3D version of OPS as the 3D dispersion model (see below for more information on the models). Thus, regarding its volatilization part BROWSE can be considered as an extension of the previous efforts because it combines a mechanistic volatilization model with an advanced 3D-dispersion model allowing flexible assessment of dispersion of plant protection products. The calculated vapour exposure is combined with exposure to spray drift, which is assessed in another component of BROWSE (Butler Ellis et al., 2016a) to estimate a total exposure.

The PEARL model (Leistra et al., 2001; Van den Berg et al., 2016) can be used to assess the fate of pesticides in the soil-plant system and is specifically used in BROWSE to determine the volatilisation rate of plant protection products from crop or soil. The PEARL model is applied in European (FOCUS, 2009; European Commission, 2014) and Dutch (Van der Linden et al., 2004) authorization procedures for assessment of leaching of plant production products to groundwater. Since 2001, the PEARL model has been developed further to include a description of the fate of the plant production products on the canopy. Relevant processes that can be taken into account include volatilisation from the leaf surface, penetration into the plant tissue, transformation under the influence of sunlight and wash-off of pesticides by canopy drip due to rainfall. The model has an option to consider the effect of hourly variation in meteorological conditions on these processes.

OPS is an atmospheric dispersion model developed by the National Institute for Public Health and the Environment (RIVM) in the Netherlands. The OPS model simulates the atmospheric process sequence of dispersion, transport, chemical conversion and finally deposition of various well-known pollutants in the air, such as ammonium, sulphur dioxide, ozone, particulate matter and heavy metals (Van Jaarsveld, 1995; Van Jaarsveld, 2004). OPS is applied in Dutch air quality and deposition assessments at national to local scale and its results underlie Dutch national air quality reports. A special version of OPS, i.e. OPS-st, has been developed for the assessment of dispersion and deposition of air pollutants at short distances from their source, originally targeted at ammonium dispersion in cattle breeding regions and around manured fields. The dispersion, dry deposition and chemical conversion processes are

modelled like in OPS, but an essential difference is that OPS-st allows hourly concentrations to be computed, using hourly meteorological observations (Smits et al., 2005; Van Pul et al., 2008). OPS-st does not require a meteorological pre-processor. It allows hourly source strength variations to be included. Such a source may be an area source at the land surface. These characteristics render OPS-st extremely suitable for the purpose of BROWSE to assess dispersion of plant protection products. To this end we extended OPS-st to include dispersion and deposition of such products on non-target areas.

The model used in BROWSE will hereafter be referred to as PEARL-OPS. In this model OPS preprocesses meteorological data, for subsequent use in PEARL. Volatilisation of plant protection products from a crop fully covering the soil surface is then calculated using the PEARL model and this output provides the emission strength for OPS. The procedure ensures a consistent use of meteorological conditions and other boundary conditions of the models, as well as a consistent evaluation of exposure and deposition at hourly timescale (Jacobs et al., 2007).

Both the PEARL model and the OPS model have been tested separately against data from field experiments. The OPS model has been validated against observations of ammonia concentrations resulting from emission and dispersion of this substance in agricultural areas (Van Pul et al., 2008; Theobald et al., 2012). Estimation of spatial and temporal variations of the concentrations were found to be acceptable. The quality of the simulations was similar to the one of other, widely used dispersion models like ADMS (Atmospheric Dispersion Modelling System; Carruthers et al., 1994) or the AMS/EPA Regulatory Model (AERMOD; Cimorelli et al., 2002). However, the quality of the model estimates critically depends on the quality of the source strength estimates (van Pul et al., 2008).

The PEARL volatilization module has been tested using data obtained from well-defined experiments in a wind tunnel. Because radio-labelled compounds have been applied, a mass balance of the compound could be established at the end of the experiment. Leistra and Wolters (2004) tested the PEARL model against a series of experiments by Ophoff (1998); Ophoff et al. (1999) and Stork et al. (1998) with applications of fenpropimorph on beans (Phaseolus vulgaris L.), radish (Raphanus sativus L.) and sugarbeet (Beta vulgaris L). The volatilisation of the pesticide at the soil surface was described assuming a laminar boundary air layer through which the pesticide has to diffuse before it can escape into the turbulent air layer. The volatilisation could be described with a thickness of the laminar air boundary layer between 0.5 and 1.0 mm, depending on wind speed levels during the experiment. Leistra and van den Berg (2007) studied the volatilisation rates of parathion and chlorothalonil (both non-systemic compounds) after spraying of a fully grown potato crop (height 0.5 m). Parathion has a comparatively high vapour pressure (0.63 mPa at 20 °C), which results in comparatively high volatilisation rates, whereas chlorothalonil has a lower vapour pressure, 0.04 mPa at 20 °C, which results in lower volatilisation rates. In both cases, there was reasonable agreement between the calculated volatilisation fluxes and those measured. Leistra et al. (2005) calculated the volatilisation of fenpropimorph after spraying on a sugarbeet crop using the Aerodynamic and Bowen ratio methods. A detailed description of these methods have been given by (Majewski, 1999). Input data on the rate coefficients of the competing processes had already been obtained in a wind tunnel study on the volatilisation behaviour of fenpropimorph. The initial volatilisation rates could be described well by the model, but the continued volatilisation measured at 3 and 5 days after application could not be simulated without introducing a poorly exposed deposit with comparatively low rates of dissipation processes. Butler Ellis et al. (2010a) measured the volatilisation rate of fenpropidin and epoxiconazole. The vapour pressure of fenpropidin is reported to be 17 mPa at 20 °C. For epoxiconazole, different vapour pressures have been reported: $4.5\cdot 10^{-4}\,\text{mPa}$ and $1.0\cdot 10^{-2}\,\text{mPa}$ (Butler Ellis, 2012). For fenpropidin the measured and calculated fluxes were in agreement, but for epoxiconazole the fluxes were underpredicted.

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