

# ESCAPE

## A new model for the Calculation of PECsoil Dependent on FOCUS Degradation Kinetics

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### Introduction

A new version of the computer model ESCAPE (Estimation of Soil Concentrations After Pesticide applications) is presented that is able to calculate time dependent pesticide concentrations in soil for active compounds and metabolites considering all kinetics recommended by FOCUS (SFO, FOMC, HS, DFOP). ESCAPE can handle regular and irregular applications, or different soil and tillage depths. Finally, in the new version 2 also concentrations in pore water can be calculated assuming linear sorption to the soil matrix. Similar to current FOCUS leaching models like PEARL or PELMO, ESCAPE is able to process daily weather data and corrects the standard microbial degradation rate depending on current soil moisture and soil temperature.

### Conclusions

It could be demonstrated that it is principally possible to use the biphasic degradation kinetics not only when analysing degradation studies but also when calculating soil concentrations. Based on the normalised 'day length' approach temperature fluctuations could be considered also for biphasic kinetics. The calculation of pore water concentration showed that metabolite concentrations have to be expected significantly above the respective a.i. concentrations mainly if the sorption constant decreases from parent to metabolite (which is the normal case).

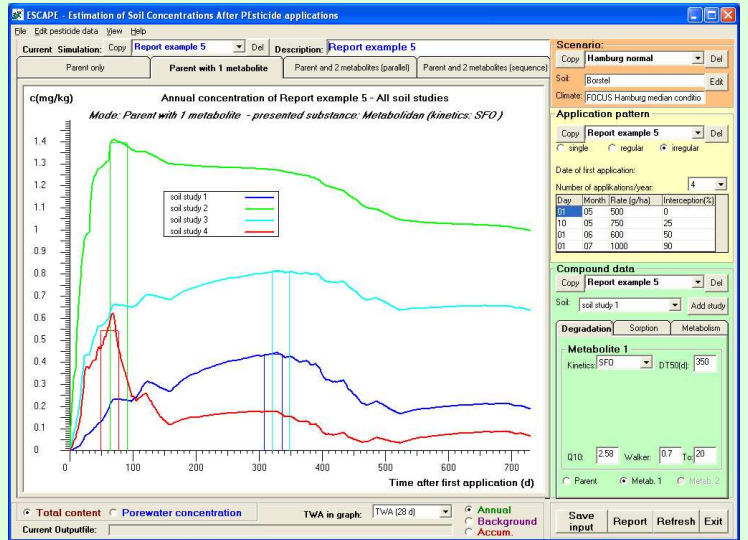
### Materials and Methods

The various degradation kinetics used by ESCAPE are generally following the methodology described in FOCUS (2006). The established temperature and soil moisture correction has been originally developed for first order kinetics only. So, for the biphasic kinetics they had to be adapted. ESCAPE uses a time-step normalisation approach to do the soil moisture and temperature correction independent on the actual degradation kinetics based on daily variations in soil temperature and moisture content. Pore water concentrations are calculated according to the following equation

$$C_{PW} = \frac{C_T}{\Theta + \frac{C_{org} K_d}{\rho}}$$

$C_{PW}$ : pore water concentration (mg/L)  
 $C_T$ : total content in soil (mg/kg)  
 $C_{org}$ : organic carbon content in soil (%)  
 $K_d$ : sorption constant (L/kg)  
 $\rho$ : soil density (kg/m<sup>3</sup>)  
 $\Theta$ : actual soil moisture (m<sup>3</sup>/m<sup>3</sup>)

Depending on the degradation model it may be important whether or not residues from different applications are kept separately. Therefore, 3 variations were implemented in ESCAPE: "yes", "no", and "yes, but only within a year" (default).



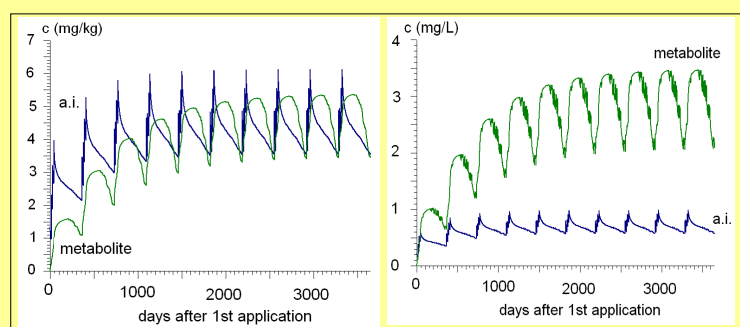
### Results of test simulations

The simulations in the figures were performed with pesticide input data as summarised in **Table 1**. The annual application pattern was 4 × 1 kg/ha (interval 14 days, start in September, no crop interception). The scenario information (soil data, daily weather series) was taken from the EU-FOCUS groundwater scenario "Hamburg". The ecological relevant concentration was 5 cm (no tillage).

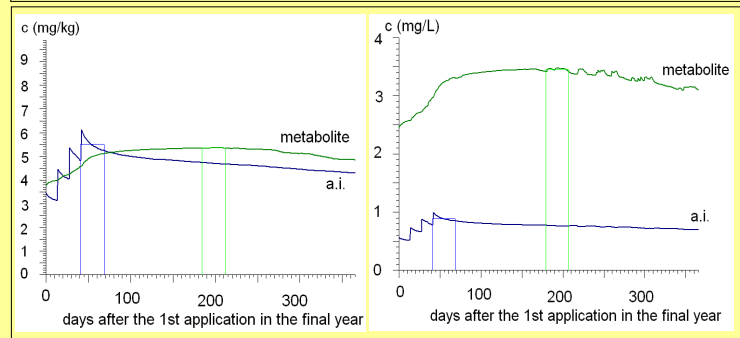
Parameter	Parent	Metabolite
Formation fraction (%)	-	80
Molar mass (g/mol):	250	200
KOC (L/kg):	400	100
Degradation model:	FOMC	DFOP
Degradation constants:	$\alpha = 0.2$ $\beta = 1$	DT50 <sub>1</sub> = 70 d DT50 <sub>2</sub> = 140 d g = 0.5

**Fig 1** demonstrates the building of the plateau for parent and metabolite caused by the annual applications. The total contents in soil shown in **Fig 2** are similar for both compounds because of the high formation fraction and persistence of the metabolite. However, pore water concentrations for the metabolite are simulated three times above respective concentrations for the parent compound (**Fig 2 right**) which can be explained by differences in the sorption constants.

Compared to the concentration in soil the pore water concentrations show additional fluctuations because they are directly influenced by soil moisture contents which change dependent on the daily weather conditions.



**Fig 1:** Time dependent concentration of parent (blue line) and metabolite (green line) in total soil (left figure) and pore water (right figure) over the first 10 years



**Fig 2:** Time dependent concentration and PECTwa (28 d) of parent (blue line) and metabolite (green line) in total soil (left figure) and pore water (right figure) in the final year.