

EPAT – An Exposure Pattern Analysis Tool

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Abstract

The behaviour of pesticides in water bodies adjacent to a single field is calculated for the registration in the EU with the surface water model FOCUS TOXSWA. The calculated pesticide concentrations in the water and sediment layer describe the exposure over time, which is typically characterized by rather short exposure peaks. The complete and very detailed information included in TOXSWA output files (*.cwa files) is currently not further analyzed. However, *.cwa files could be of considerable use, specifically for analysis of how often a given concentration is reached or how long a concentration may be expected to remain above a given threshold. Such results may be useful for refined estimates of the acute or chronic risk (see E-LINK workshop, Brown & Asshauer 2007). For this purpose a new program (EPAT, Exposure Pattern Analysis Tool) was developed. EPAT is an evaluation tool specifically designed for the analysis of TOXSWA output files but can also be used for other concentration time series data in aquatic, terrestrial or other environmental compartments. EPAT analyses how long an exposure above a certain level is observed and which maximum concentrations or peaks are reached. The analysis of exposure events may be regarded relevant for the estimation of the chronic risk of an organism (e.g. how long an exposure above a given NOEC is observed), while the analysis of maxima or peaks may be applied as a measure of the acute risk.

EPAT and a program manual can be downloaded at: http://rifcon.de/index.php?id=102

Introduction

Time-variable surface water exposure profiles of pesticides are more often the rule rather than the exception. FOCUS simulations are able to reproduce the general characteristics of measured pesticide concentrations in the water column of edge-of-field water bodies (streams, ditches, ponds) and are widely used in aquatic exposure assessment in the EU. However, only the maximum concentrations and the time weighted average concentrations up to 100 days after the maximum peak are currently used in pesticide exposure assessments in the EU evaluation process, although FOCUS simulations produce much more detailed results. Specifically, the FOCUS model TOXSWA produces detailed time-variable concentration profiles. These could be used for risk assessments to examine how often a given concentration is reached or how long a concentration may be expected to remain above a given threshold. Such results may be useful for refined estimates of both the acute and chronic risk (see E-LINK workshops, Brown & Asshauer 2007, www.elinkinfo.org). To characterize the complex exposure profiles simulated for stream, ditch and pond environments, metrics or parameters that allow a description of different exposure profiles are proposed by the E-LINK-workshops (www.elink-info.org). These parameters that describe exposure characteristics, can be used to delineate exposure regimes for highertier effects studies. For obtaining these metrics or parameters an evaluation tool (EPAT, Exposure Pattern Analysis Tool) was developed (figure 1). Special emphasis was given to facilitate the analysis of time-variable exposure patterns calculated by TOXWSA. However other, user defined concentration patterns can also be considered.

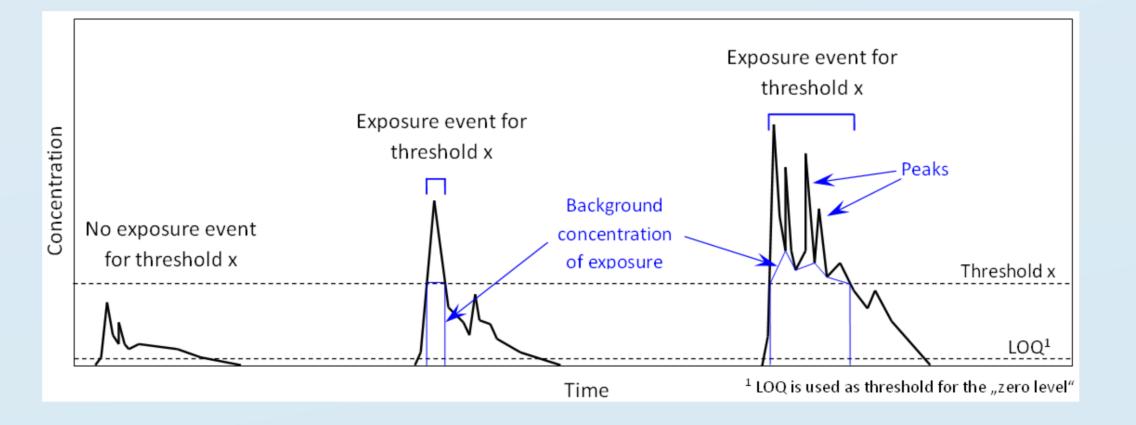
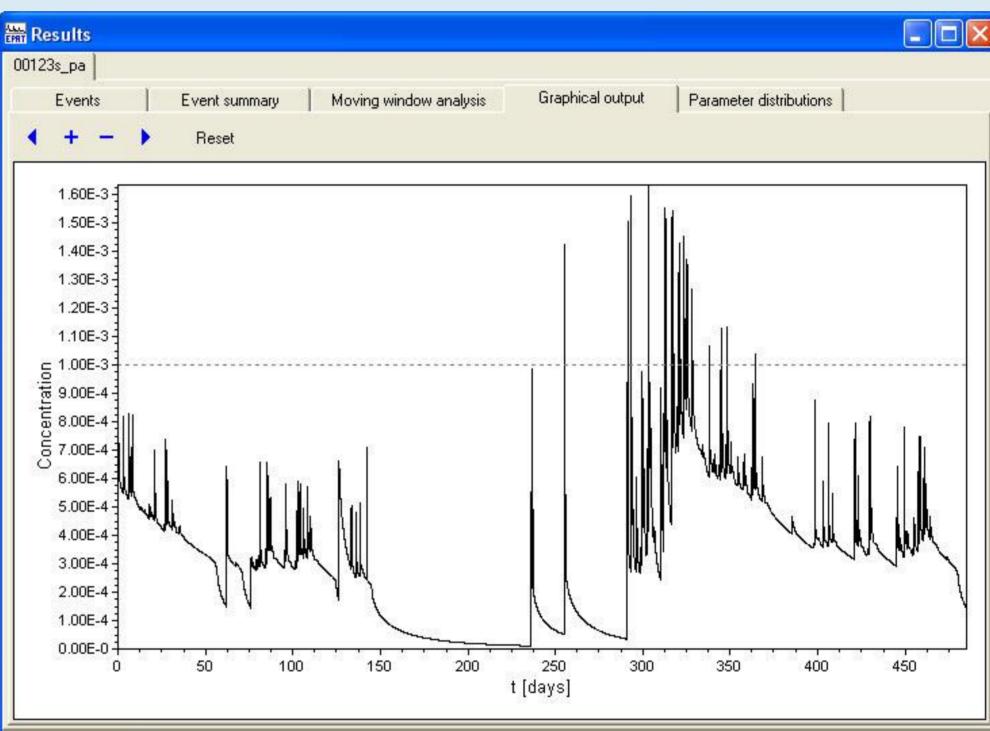


Figure 2. Definition of exposure events (concentration above a given threshold), peaks and the background concentration (blue lines) calculated in EPAT.

The key exposure parameters calculated by EPAT are:

Height of concentration peaks



- Area under the curve (AUC) concentrations
- Duration of exposure peaks
- Interval between peaks
- Height of a possible long-term background concentration
- Frequency of peaks
- Time weighted average (TWA) concentrations

EPAT analyses "exposure events". Events are defined as periods during which pesticide concentrations exceed a given threshold. One or more thresholds can be defined by the user (additionally, events are always analysed for a limit of quantification, LOQ, used as a "zero level"). An illustration of the concept of exposure events is shown in figure 2.

EPAT calculates all parameters for each event, such as the maximum concentration, the number of extrema, the area under the curve, the TWA or the interval since the previous event.

| Results | | | | | | Results | | | | | |
|-----------------------|---------------|---------------------------|------------------|------------------------|----------------|--------------------|---------------------|-------------------|------------------------|------------------------------|-----|
| 0123s_pa | | | | | | 00123s_pa | | | | | |
| Events | Event summary | Moving window analysis | Graphical output | Parameter distribution | s | Events | Event summary | Moving window | v analysis Graphical o | utput Parameter distributi | ons |
| Threshold conc. | Event no. | Start date & time t [d | ay] Max.o | onc. Duration | [days] Interva | Window size [days] | Percentile | AUC | TWAC | | 8 |
| 1.000e-05 (zero level |) 1 🕳 | 01.01.1986 01:00:00 0.0 | 42 1.635 | e-03 484.958 | · . | 1 | Max | 2.694e-02 | 1.123e-03 | 1 | |
| 5.000e-04 | 1 | 01.01.1986 01:00:00 0.0 | 42 8.778 | e-04 12.041 | | 1 | Min | 2.618e-04 | 1.091e-05 | 1 | |
| .000e-04 | 2 | 14.01.1986 06:00:00 13. | 250 5.011 | e-04 0.167 | 1.167 | 1 | 10th | 6.701e-04 | 2.792e-05 | 1 | |
| .000e-04 | 3 | 10.01.1000.00.00.00 10 | 105 5100 | - 04 0.000 | 4.708 | 1 | 25th | 2.500e-03 | 1.042e-04 | 1 | |
| .000e-04 | 4 | Eirot o | | avant fa | 2.917 | 1 | 50th | 7.915e-03 | 3.298e-04 | 1 | |
| 5.000e-04 | 5 | riist a | na oniy | event fo | 5.750 | 1 | 75th | 1.048e-02 | 4.365e-04 | 1 | |
| 5.000e-04 | 6 | | • | | 0.625 | 1 | 90th | 1.474e-02 | 6.140e-04 | 1 | |
| 5.000e-04 | 7 | thres | hold 1.0 | 00e-05 | 2.792 | 1 | 95th (user defined) | 1.706e-02 | 7.107e-04 | | |
| .000e-04 | 8 | | | | 30.95 | 2 | Max | 4.983e-02 | 1.038e-03 | 1 | |
| 5.000e-04 | 9 | 23.03.1986 03:00:00 81. | 125 6.566 | e-04 0.250 | 18.7% | 2 | Min | 5.275e-04 | 1.099e-05 | | |
| 5.000e-04 | 10 | 27.03.1986 03:00:00 85. | 125 6.600 | e-04 0.333 | 3.750 | 2 | 10th | 1.353e-03 | 2.819e-05 | | |
| .000e-04 | 11 | 28.03.1986 03:00:00 86. | 125 6.111 | e-04 0.167 | 0.667 | 2 | 25th | 5.125e-03 | 1.068e-04 | | |
| .000e-04 | 12 | 29.03.1986 03:00:00 87.1 | 125 5.339 | e-04 0.083 | 0.833 | 2 | 50th | 1.604e-02 | 3.341e-04 | | |
| 5.000e-04 | 13 | | | | 8.959 | 2 | 75th | 2.091e-02 | 4.356e-04 | 5 | |
| 5.000e-04 | 14 | Sixth A | vent for | threshol | d 6.875 | 2 | 90th | 2.903e-02 | 6.048e-04 | | |
| 5.000e-04 | 15 | Sixth event for threshold | | | 0.792 | 2 | 95th (user defined) | 3.364e-02 | 7.009e-04 | | |
| .000e-04 | 16 | | 5.000e- | $\cap I$ | 3.834 | 4 | Max | 9.520e-02 | 9.917e-04 | | |
| .000e-04 | 17 | | 5.000e- | 04 | 18.04; | 4 | Min | 1.071e-03 | N16e-05 | | |
| 000e-04 | 18 | 14.05.1986 11:00:00 133 | 3.458 5.054 | e-04 0.125 | 5.875 | 4 | 10th | 2 702- 02 | 2.07 05 | | |
| .000e-04 | 19 | | 3.208 5.160 | | 4.625 | 4 | 254 | 41- | | | |
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|--|---|
| Events Event summary Moving window analysis Graphical output Parameter distributions select threshold level: 5.000e-04 Show distribution of: TWAC Values: 22 TWAC 1 5.789E-04 2 5.008E-04 24 0 1 5.789E-04 2 5.008E-04 24 0 1 5.789E-04 2 5.008E-04 25 5.008E-04 3 5.101E-04 4 6.041E-04 36 6.079E-04 7 5.234E-04 8 5.871E-04 21 10 6.051E-04 10 6.051E-04 | |
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| TWAC TWAC 22 5.008E-04 20 5.101E-04 10 6.079E-04 2 5.001E-04 4 6.041E-04 5 6.662E-04 6 6.079E-04 7 5.234E-04 8 5.871E-04 9 5.961E-04 10 6.051E-04 | |
| TWAC 1 5.789E-04 22 5.008E-04 3 5.101E-04 20 4 6.041E-04 5 6.662E-04 16 6 6.079E-04 7 5.234E-04 14 8 5.871E-04 9 5.961E-04 2 10 6.051E-04 10 6.051E-04 | |
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| 22 20 18 16 14 2 12 2 12 3 5.101E-04 4 6.041E-04 5 6.662E-04 6 6.079E-04 7 5.234E-04 8 5.871E-04 9 5.961E-04 10 6.051E-04 | |
| 20 18 16 14 212 10 10 10 10 10 10 10 10 10 10 | |
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Figure 4. Graph of an exposure time series (top) and histogram of the distribution of a parameter (here time weighted average concentration,TWAC, bottom).

9.00E-4

1.00E-3

5.544E-04

5.590E-04

5.669E-04

5.030E-04

5.097E-04

20 7.092E-04

Additionally, for all events global maximum concentrations, median values and percentiles are calculated. Sample outputs are shown in figure 3. The concentration profile can also be shown graphically, together with the selected thresholds which define an event, and parameter distributions can be displayed as histograms (figure 4).

| General settings Evaluation genod. Complete series Image: Complete ser | <u>File A</u> nalysis Info | | | |
|--|---|--|---------|---------------|
| Evaluation geriod: Complete series: Image: Complete series: <td< th=""><th>Image: Second state Image: Second state Image: Second state Image: Second state</th><th></th><th></th><th></th></td<> | Image: Second state Image: Second state Image: Second state Image: Second state | | | |
| Evaluation period Complete series Start [d] Start [d] Image: Start [d] Image: Start [d] | General settings | Files selected for analysis | | |
| End [d]: 365 Assumed LOQ: 11000E-10 (used as "zero-level") Please enter thresholds using the same unit as they are given in your input file(s), e.g. g/m in TOXSWA cwa." files. Threshold concentration 1 2 3 4 5 6 7 Wiscellaneous settings User defined percentile: 95 Output directory | | A state of the second se second second s second second se | | |
| (used as "zero-level") Threshold concentrations Please enter thresholds using the same unit as they are given in your input file(s), e.g. g/m² in TOXSWA cova." files. Threshold concentration 1 2 3 4 5 6 7 Miscellaneous settings User defined percentile: 95 Output directory | | Filename | Segment | Add file |
| Threshold concentrations Please enter thresholds using the same unit as they are given in your input file(s), e.g. g/m² in TOXSWA cwa." files. Threshold concentration 1 2 3 4 5 6 7 | Assumed LOQ: 1.0000E-10 | | | Delete file |
| Please enter thresholds using the same unit as they are given in your input file(s), e.g. g/m² in TOXSWA cwa.* files. Image: | (used as "zero-level") | | | |
| they are given in your input file(s), e.g. g/m² in Image: Strategy of the st | Threshold concentrations | | | |
| Image: settings User defined percentile: 95 Output directory | Please enter thresholds using the same unit as they are given in your input file(s), e.g. g/m³ in TOXSWA cwa.* files. | | | |
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| 4 5 6 7 Miscellaneous settings User defined percentile: 95 Output directory | | | | |
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Figure 1. The Graphical User Interface (GUI) of EPAT.

Functionality

EPAT works either with one or more (batch simulations) surface water concentration files, generated by the FOCUS model TOXSWA, or with surface water concentration time series (hourly and daily time resolutions) prepared by the user (e.g. monitoring data).

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|------------------------|--|---------|---|-------------------------------------|-------------|--|--------------|-----------------|--------|--|
| Events | Events Event summary reshold conc. No. events 000e-05 (zero level) 1 | | Moving window an | alysis | Graphical o | output Parameter distributions | | | | |
| Threshold conc. | | | Percentile | Max. conc. | \$9 | Duration | [days] | Interval [days] | No. ex | |
| 1.000e-05 (zero level) | | | Max | 1.635e-03 | | 484.958 | | - | 162.0(| |
| 1.000e-05 (zero level) | 1 | | Min | 1.635e-03 | | 484.958 | | | 162.00 | |
| 1.000e-05 (zero level) | 1 1 1 1 1 | | 10th | 1.635e-03 1.635e-03 1.635e-03 | | 484.958 484.958 484.958 | | - | 162.00 | |
| .000e-05 (zero level) | | | 25th | | | | | | 162.00 | |
| .000e-05 (zero level) | | | 50th | | | | | | 162.00 | |
| .000e-05 (zero level) | | | 75th | 1.635e-03 | | 484.958 | | | 162.00 | |
| .000e-05 (zero level) | | | 90th | 1.635e-03 | | 484.958 | | • | 162.00 | |
| 1.000e-05 (zero level) | | | 95th (user defined) | 1.635e-03 | | 484.958 | | 1 | 162.00 | |
| 5.000e-04 | | | Max 1.635e-03 | | | 56.084 🛓 | | 93.916 | 33.00(| |
| 5.000e-04 | 48 | | Min | 5.011e-04 | | 0.042 | \backslash | 0.209 | 1.000 | |
| 5.000e-04 | 48 | | 10th | 5.189e-04 | | 0.083 | \backslash | 0.633 | 1.000 | |
| 5.000e-04 | 48 | Mox o | oncontration | 5.854e-04 | | Max overt | | otion | 1.000 | |
| 5.000e-04 | 48 48 48 events o | | oncentration ved over 48 defined by a | 6.821e-04 | | Max. event d observed ov events define | | | 1.000 | |
| 5.000e-04 | | | | 8.485e-04 | | | | | 1.000 | |
| 5.000e-04 | | | | 1.483e-03 | | | | | 1.000 | |
| 5.000e-04 | 48 | thresho | ld of 5.0e-04 | 1.557e-03 | +03 thresho | | old of 5.0 |)e-04 | 2.400 | |
| 1.000e-03 | 18 | | Max | 1.635e-03 | | 0.542 | | 35.708 | 1.000 | |
| 1.000e-03 | 18 | | Min | 1.037e-03 | | 0.041 | | 0.458 | 1.000 | |
| 1.000e-03 | 18 | | 10th | 1.086e-03 | | 0.138 | | 0.633 | 1.000 | |
| 1.000e-03 | 18 | | 25th | 1.163e-03 | | 0.250 | | 0.740 | 1.000 | |
| 1.000e-03 | 18 | | 50th | 1.428e-03 | | 0.292 | | 2.542 | 1.000 | |
| | | | | 4 540 00 | | 0.075 | | 0.054 | 4 000 | |
| | | | | | | | | | | |

Figure 3. Example output produced by EPAT: Analysis of events (top left), moving window analysis (top right) and event summary (bottom).

Conclusions

6.00E-4

<u>C</u>lose

7.00E-4

8.00E-4

EPAT makes it possible to analyse the exposure profile in water or sediment after application of pesticides in great detail, revealing how long or how often given concentrations are reached or surpassed. These analysis can give relevant information for the estimation of the chronic risk of an organism (e.g. how long an exposure above a given NOEC is observed), or for a refined estimation of the acute risk (e.g. when or how maxima or peaks are observed).

Acknowledgements

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References

Brown, C. and Asshauer, R. 2007, E-Link Workshop Report, ECO-FRAM guidance document.