



FERTILIZERS ENVIRONMENTAL EXPOSURE (FEE) TOOL

User guidance for environmental exposure assessment of fertilizers under REACH

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DISCLAIMER

The Fertilizers Environmental Exposure (FEE) tool has been developed to aid users in the environmental exposure assessment of fertilizers, soil improvers and related products. The tool is made freely available on the Fertilizers Europe website <http://www.reachfertilizers.com/>. In the FEE tool, environmental fate calculations are based upon equations from the REACH R.16 Guidance document (ECHA, 2016) and complemented with calculation methods and parameters from Steps 1-2 in FOCUS (FOCUS, 2015) and Simplebox (the regional REACH environmental exposure model; RIVM, 2014) where required. Great care has been taken in programming this software tool, using detailed comparison with the above mentioned guidance documents. Nevertheless, flawless operation cannot be guaranteed. The content of the spreadsheets within the tool must not be modified by the user. By using the FEE tool, users accept full responsibility for their calculations. The producers of this spreadsheet cannot take liability for any use or misuse of the results.

1. INTRODUCTION

In order to comply with the requirements of European Regulation (EC) No. 1907/2006 (REACH), a chemical safety assessment needs to be performed for substances manufactured or imported above 10 tonnes/year. Fertilizers are considered as formulations and therefore no registration or chemical safety assessment is required for fertilizers as such under REACH. However, the use of the individual constituents needs to be covered in the Chemical Safety Report (CSR) of the substances. Currently the exposure and risk assessment of fertilizer uses is mainly described in a qualitative way because the lack of appropriate environmental release categories (ERC's) and exposure models for fertilizer use.

As a first step, after extensive use mapping of the main fertilizer uses under the umbrella of Fertilizers Europe and FARM (REACH consortium of manufacturers of Fertilizers and Related Materials), specific ERC's (SPERC's) were developed. For each group of similar uses, realistic emission rates to air, water and soil were derived taking into account different methods of application (e.g. foliar spraying, direct application into/onto soil) and product properties (solids, granules, liquids). The development of the **SPERCs** for the main fertilizer use categories is described in detail in Chapter 1.1.

Secondly, a **Fertilizers Environmental Exposure (FEE) tool** was developed for environmental fate modelling of fertilizer substances and soil improvers, since in the standard REACH models for environmental exposure assessment (EUSES, ECETOC TRA, CHESAR), no local scenario for direct emissions to soil exists. Quantitative exposure scenarios, resulting in the calculation of realistic worst-case Predicted Environmental Concentrations (PECs) for fertilizer constituents in the various environmental compartments (soil, water, sediment) were established. General aspects of development and design of the FEE tool are described in Chapter 1.2. Chapter 2 of this document provides practical guidance, in the form of a user manual, for environmental exposure assessment of fertilizer substances, soil improvers and related products, using the FEE tool.

The FEE tool is recommended for use in quantitative environmental exposure assessment of fertilizer compounds instead of the standard REACH models.

1.1. FERTILIZERS EUROPE SPERCS

The standard approach for environmental exposure assessment under REACH is to select the most appropriate Environmental Release Category (ERC) for each use, as described in Chapter R.16 of the REACH Guidance on Information Requirements & Chemical Safety Assessment (ECHA, 2016). These ERCs are defined as generic, broadly applicable emission scenarios. They define the fractions of a substance emitted to the various environmental compartments, and provide default assumptions for standardized local environmental properties.

ERC8e, referring to widespread use of reactive processing aids (no inclusion into or onto article; outdoor) was selected as the most relevant ERC for outdoor use of fertilizer nutrients by Fertilizers Europe uses map work. However, ERC8e emission estimates reflect the process of losses to the environment from the local use of substances, but does not reflect emissions to soil, water and air through direct application. Furthermore, although ERCs provide for standardization, they often lead to unrealistic emission estimates. The REACH R.16 guidance acknowledges that an “ERC should be used as a starting point for emission estimation” and explicitly encourages the use of more refined or specific information on emissions, resulting in the development, and use of specific ERCs (SPERCS).

Based on extensive use mapping of fertilizer applications, the uses were grouped towards common emission potential to the environment and corresponding SPERCS were developed for each group. These SPERCS are used to specify broad emission scenarios, as defined in the ERCs. Even though they are more specific, SPERCS still describe emission scenarios applicable to a wide range of substances within an industry sector, and are intended to represent conservative estimates of environmental exposure (Reihlen et al., 2016).

For the outdoor application of fertilizers and related products, four different SPERCS have been developed. SPERC 1 (Fertilizers Europe SPERC 8e.1.v1), SPERC 2 (Fertilizers Europe SPERC 8e.2.v1) and SPERC 4 (Fertilizers Europe SPERC 8e.4.v1) can be used to assess the exposure of both professional and consumer fertilizer uses. SPERC 3 (Fertilizers Europe SPERC 8e.3.v1) is applicable only to professional fertilizer users. Grouping was mainly based on the physical form of the fertilizers and their mode of application (Table 1).

Table 1. SPERCS for professional and consumer uses of fertilizer substances

| SPERC number | SPERC code | Title | Application area |
|--------------|----------------------------------|--|--|
| SPERC 1 | Fertilizers Europe SPERC 8e.1.v1 | Outdoor use - direct application of solid fertilizers to soil; surface spreading | Professional and consumer use of nutrients in solid granular fertilizers, applied onto soil surface with or without crop cover. |
| SPERC 2 | Fertilizers Europe SPERC 8e.2.v1 | Outdoor use - direct application of solid or liquid fertilizers to soil; incorporation, placement, mixing, seed treatment, drip irrigation | Professional and consumer use of nutrients in solid and liquid fertilizers. Fertilizers become either placed into soil, ploughed into soil or will penetrate into soil when using fertigation dripping system. |
| SPERC 3 | Fertilizers Europe SPERC 8e.3.v1 | Outdoor use - application of fertilizers by helicopter | Professional use of nutrients in fertilizers. Spreading happens from helicopter. |
| SPERC 4 | Fertilizers Europe SPERC 8e.4.v1 | Outdoor use - spray application of liquid fertilizers; soil surface spreading, sprinkler, pivot, foliar spray, slurry | Professional and consumer use of nutrients in liquid fertilizers. |

The Fertilizers Europe SPERCs cover local scale, widespread use of solid and liquid fertilizers, soil improvers and related products in crop growing by professionals and consumers. Farmers are considered professional users. The SPERCs are focused on outdoor uses in an agricultural setting, including use in a.o. forestry, horticulture, gardens and golf courses. They also cover the use of fertilizers in covered structures when crops are cultivated in contact with the soil (e.g. non-permanent covers, walk-in tunnels and nurseries). In this case, outdoor use represents a worst-case for environmental exposure. High-tech greenhouse structures, with no direct soil contact and closed water circulation systems are excluded from the Fertilizers Europe SPERCs .

The Fertilizers Europe SPERCs cover both the application stage, as well as the mixing and loading step of the fertilizer uses. Emissions from the formulation and re-packaging at industrial manufacturing sites are not addressed by the Fertilizers Europe SPERCs. More detail on the different Fertilizer Europe SPERCs and their release factors can be found in the **SPERC background document** (Fertilizers Europe, 2017).

1.2. FEE TOOL

In the standard REACH models for environmental exposure assessment (EUSES, ECETOC TRA, CHESAR), no local emission scenario for direct application to soil exists. In addition, the default local environmental exposure assessment for REACH does not take into account several processes that are important for the environmental fate of fertilizer constituents, e.g. plant uptake with subsequent crop harvest or losses via spray drift and transfer from soil surface to surface water at the local scale via runoff or drainage. Therefore, an Excel based exposure tool was developed for local environmental fate modelling of fertilizer substances: the Fertilizer Environmental Exposure calculation (FEE) tool. The main focus of the FEE tool is on fertilizer micronutrients such as manganese, copper and zinc, which are identified as hazardous for the aquatic environment; but the tool allows for the assessment of other inorganic and organic substances as well.

Further information on this project, including downloads of the SPERC factsheets and the FEE tool, can be found on the website of Fertilizers Europe <http://www.reachfertilizers.com/>

The FEE tool is recommended to be used in quantitative environmental exposure assessment of fertilizer compounds instead of the standard REACH models.

2. USER GUIDANCE FEE TOOL

2.1. GENERAL ASPECTS

In the FEE tool, environmental fate calculations are based upon equations from the REACH R.16 Guidance document (ECHA, 2016) and complemented with calculation methods and parameters from Steps 1-2 in FOCUS (a validated first tier model used for environmental exposure assessment of plant protection products; FOCUS, 2015) and Simplebox (the regional REACH environmental exposure model; RIVM, 2014) where required.

The local scenario for environmental exposure assessment in the FEE tool is based upon the standard exposure scenario in the 'Steps 1-2 in FOCUS' model: a 1 ha agricultural field, surrounded by a shallow water body (width of 2.5 m and depth of 0.3 m), with a surface of one tenth of the agricultural field (field:water ratio of 10). Assuming a 1 ha field, the 0,1 ha water body has a volume of 3×10^5 liters.

For environmental exposure assessment of fertilizers, a number of parameters or processes are important in determining emissions to the various environmental compartments (soil, surface water and sediment). In the FEE tool, depending on the SPERC, the following processes are included for calculating the Predicted Environmental Concentrations (PECs): drift, runoff and crop offtake, leaching, volatilization and degradation. Crop growth stage (BBCH stages; determining crop interception) can be introduced and reduces the fraction available for runoff (Chapter 2.2.2; Table 2).

| SPERC | Drift | Runoff | Crop interception | Crop offtake | Leaching | Volatilization | (Bio-) degradation |
|-------------|-------------|------------|-------------------|----------------|------------|----------------|--------------------|
| SPERC 1 | | X | | X | X | X | X |
| SPERC 2 | | | | X | X | X | X |
| SPERC 3 | X | X | X | | X | X | X |
| SPERC 4 | X | X | X | X | X | X | X |
| Data source | Focus, 2015 | RIVM, 2014 | EFSA, 2014 | Eurostat, 2016 | ECHA, 2016 | ECHA 2016 | ECHA, 2016 |

Fig. 1 Overview of the important processes for local environmental fate calculations of the different SPERCs.

In the next paragraphs, practical guidance is presented on how to use the tool (Chapter 2.2). Defaults and specific processes used in the PEC calculations are presented (Chapter 2.3). And details on the outcome of the environmental fate calculations, regarding safe use of the substance in a specific scenario and corresponding risk characterisation ratios (RCRs) are described (Chapter 2.4).

In this guidance document, references to specific tables and equations from existing exposure models are indicated in **green** for easy cross-referencing.

2.2. RUNNING THE FEE TOOL: BASIC AND REFINED ASSESSMENT

As a first step, environmental exposure can be calculated by the FEE tool for the various compartments (soil, water and sediment), using the default release fractions from the Fertilizers Europe SPERCs (Chapter 1.1), plus selection of a “Generic crop”. Refinement options can be made by including the choice of a specific crop, growth stage and yield scenario, in order to refine drift and runoff estimates, and include crop offtake by harvest. On a case-by-case basis, if needed, also risk management measures (drift reduction) can be included in a final step.

2.2.1. BASIC ASSESSMENT

The FEE tool has been made available as an Excel based tool. Input parameters needed in order to run the FEE tool should to be entered or selected in the sheet ‘Input’. Minimum required input fields for a basic environmental exposure assessment are indicated in green (Fig. 2).

| | |
|--|---|
| 1. Substance | Copper |
| 2. Specific Environmental Release Category (SpERC) | SpERC 1: Outdoor use - solid application; surface spreading |
| 3. Single or multiple applications per growing season? | Single |
| Total annual fertilizer use rate | [kg/ha/year] |

Fig. 2 Input for default environmental assessment in the FEE tool (mandatory input fields)

SUBSTANCE SELECTION

As first step the substance to be assessed needs to be specified. This can be done by selecting from the drop down menu one of the micronutrients copper, zinc or manganese. There is also the option to select ‘Other’, if the user wishes to use the tool for environmental exposure assessment of any other inorganic or organic substance used as fertilizer or soil improver.

For the three micronutrients (Cu, Zn, Mn) standard substance properties and parameters from the REACH dossiers (phys-chem endpoints, PEC_{regional} and PNECs for the different environmental compartments) are already included in the tool, and will be shown automatically in the ‘Standard parameters’ fields of the ‘Substance properties’ table in the tool (light green fields). These standard parameters for micronutrients are based upon information from the REACH dissemination website (unless otherwise stated) and should be checked carefully by the user of the FEE tool for consistency with the most recent dossier information. If needed (e.g. when more specific or up-to-date information is available) these standard parameters can be overwritten in the ‘Refined parameters’ column of the table (light blue fields).

In case the substance 'Other' is selected from the drop down menu, manual input of substance parameters is required in order to run the FEE tool. In case of missing input fields, an error message will be shown. Substance specific information should be entered in the 'Refined parameters' (light blue) column of the 'Substance properties' table.

CHOICE OF SPERC

The second input field is a drop down menu from which the most appropriate Fertilizer Europe SPERC can be selected (cf. Chapter 1.1, Table 1), depending on the application technique and properties of the fertilizer substance. These four SPERCs are based upon extensive use mapping and cover the main fertilizer use categories for professional and consumer use. It is not possible to perform an environmental assessment using the FEE tool for uses that fall outside the scope of these listed SPERCs.

APPLICATION PATTERN

By default, it is assumed that the fertilizer is applied in one single application ('Single' selected from the drop down menu). In this case, only the total annual fertilizer use rate (in kg/ha/year) needs to be entered.

If there are multiple applications per growing season, 'Multiple' needs to be selected from the drop down menu (Fig. 3). In this case, the number of applications and the time between applications (in days) also needs to be entered into the respective fields. The FEE tool will automatically calculate the Fertilizer use rate per application (kg/ha).

| | | |
|--|----------|--------------|
| 3. Single or multiple applications per growing season? | Multiple | |
| Total annual fertilizer use rate | 6,00 | [kg/ha/year] |
| Number of applications | 2 | - |
| Time between applications | 10 | [days] |
| Fertilizer use rate per application | 3,00 | [kg/ha] |

Fig. 3 Input fields in case of multiple applications per growing season

When a basic assessment is performed, as default input a conservative generic crop type (i.e. no removal by crop offtake) is being simulated, at early growth stages (bare soil, BBCH 00-09) (Fig 4). In a refined assessment these defaults can be adjusted and risk management measures can be included on a case-by-case basis if required; this is further described in paragraph 2.2.2.

2.2.2. REFINED ASSESSMENT

In the FEE tool there are a number of refinement options possible: choice of a specific crop type, crop growth stage and European yield scenario can be selected from pre-defined drop down menu's (Fig. 4).

| | |
|------------------------------|-----------------------|
| 4. Refinement options | |
| Crop type | Generic crop |
| Crop growth stage (BBCH) | Bare soil, BBCH 00-09 |
| European crop yield scenario | Low |
| Crop substance concentration | [g/t] |
| Crop yield | [t/ha] |

Fig. 4 Input fields for refined assessment (non-mandatory input fields)

CROP TYPE

In the default exposure assessment, a generic crop type is selected. This generic crop is linked to default, conservative values for spray drift depending on the selected SPERC (Table 2; for details on selected drift values refer to SPERC background document; Fertilizers Europe, 2017) and to absence of crop offtake during harvest (conservative scenario). Different crop types can be selected for a refined exposure assessment, based upon the FOCUS crops as listed in 'Steps 1-2 in FOCUS' (Table 3; FOCUS, 2015). For SPERC 4, the choice of a specific crop type is linked to a specific drift value: ranging from 2.8% for field crops, to 29.2% for pome/stone fruit, late application. This is in agreement with the Rautmann drift values as used in 'Steps 1-2 in FOCUS' (Table 3; FOCUS, 2015; Rautmann et al, 2001). These crop specific drift values are related to a minimum distance of 1-3m from the edge of the field to the water body. For all SPERCs, the selected crop type is used for calculation of crop offtake.

Table 2. SPERC specific drift values and crop growth stage dependent runoff reduction ("generic crop")

| | Drift (%)* | Crop growth stages (BBCH codes) [% runoff reduction] | | | |
|---------|------------|--|--------------------------------|-------------------------------------|-------------------------|
| SPERC | | Bare soil, BBCH 00-09 | Minimal crop cover, BBCH 10-19 | Intermediate crop cover, BBCH 20-39 | Full canopy, BBCH 40-89 |
| SPERC 1 | 0 | 0 | 10 | 25 | 40 |
| SPERC 2 | 0 | 0 | 0 | 0 | 0 |
| SPERC 3 | 33.2 | 0 | 20 | 50 | 70 |
| SPERC 4 | 15.7 | 0 | 20 | 40 | 65 |

*Since in the respective agricultural scenario only 1/10th of the agricultural field is assumed to contribute to drift (edges of the field), actual drift values used in the calculations are divided by 10.

CROP GROWTH STAGE

As the default crop growth stage, 'Bare soil, BBCH 00-09' is selected as worst-case. This can be refined, where relevant, by choosing different crop growth stages (based on BBCH codes). These crop growth stages are linked to the calculation of runoff from the agricultural field to the adjacent water body; i.e. no reduction in runoff (0%) when fertilizers are applied to bare soil, up to 70% reduction in case of application on full canopy (Table 2). For SPERC 1, crop shoots and root systems are assumed to reduce erosion and surface runoff. For SPERC 3 and

SPERC 4 crop canopy interception reduces the fraction reaching the soil surface, consequently reducing the fraction available for runoff. Respective runoff reduction defaults per SPERC are based upon FOCUS interception fractions for 'Vegetables bulb' (SPERC 1), 'Aerial application' (SPERC 3) and 'Pome/stone fruit (late)' (SPERC 4) as realistic worst-case defaults (EFSA, 2014; Table 3). For SPERC 2, precision placement, runoff is considered not relevant since fertilizers are applied by direct placement (Table 2).

For SPERC 4, in case a specific crop type is selected the combination of crop type and crop growth stage will lead to the selection of a specific runoff reduction factor (Table 3).

Table 3. FOCUS crop types for refined assessment of SPERC 4; corresponding drift values and crop interception fractions (%) for different crop growth stages (EFSA, 2014; Focus, 2015)

| FOCUS crop | Drift (%) | Crop interception fraction (%) | | | |
|-----------------------------|-----------|--------------------------------|--------------------------------|-------------------------------------|-------------------------|
| | | Bare soil, BBCH 00-09 | Minimal crop cover, BBCH 10-19 | Intermediate crop cover, BBCH 20-39 | Full canopy, BBCH 40-89 |
| Cereals, spring | 2.8 | 0 | 0 | 20 | 70 |
| Cereals, winter | 2.8 | 0 | 0 | 20 | 70 |
| Citrus | 15.7 | 0 | 80 | 80 | 80 |
| Field beans | 2.8 | 0 | 25 | 40 | 70 |
| Grass / alfalfa | 2.8 | 0 | 40 | 60 | 75 |
| Hops | 19.3 | 0 | 20 | 50 | 70 |
| Legumes | 2.8 | 0 | 25 | 50 | 70 |
| Maize (grain) | 2.8 | 0 | 25 | 50 | 75 |
| Maize (silage) | 2.8 | 0 | 25 | 50 | 75 |
| Oil seed rape, spring | 2.8 | 0 | 40 | 70 | 75 |
| Oil seed rape, winter | 2.8 | 0 | 40 | 70 | 75 |
| Olives | 15.7 | 0 | 70 | 70 | 70 |
| Pome / stone fruit, (early) | 29.2 | 0 | 20 | 40 | 65 |
| Pome / stone fruit (late) | 15.7 | 0 | 20 | 40 | 65 |
| Potatoes | 2.8 | 0 | 15 | 50 | 70 |
| Soybeans | 2.8 | 0 | 20 | 50 | 75 |
| Sugar beet | 2.8 | 0 | 20 | 70 | 75 |
| Sunflower | 2.8 | 0 | 20 | 50 | 75 |
| Tobacco | 2.8 | 0 | 20 | 70 | 75 |
| Vegetables, bulb | 2.8 | 0 | 10 | 25 | 40 |
| Vegetables, fruiting | 2.8 | 0 | 25 | 50 | 70 |
| Vegetables, leafy | 2.8 | 0 | 25 | 40 | 70 |
| Vegetables, root | 2.8 | 0 | 25 | 50 | 70 |
| Vines, early applications | 2.7 | 0 | 40 | 50 | 60 |
| Vines, late applications | 8.0 | 0 | 40 | 50 | 60 |
| Forest (aerial application) | 33.2 | 0 | 20 | 50 | 70 |

CROP YIELD SCENARIO

Fertilizers are designed to close the gap between the natural nutrient supply of the soil and the nutrient requirement of different cultivated crops and are therefore applied if soil availability of nutrients is low. Fertilizers can contain both macro- and micronutrients that are essential for optimal plant growth (Fertilizers Europe, 2016). Nutrients are primarily (actively) taken up by the plant from soil pore water, via the plant's root system, but also via foliage for spray applications. When a plant is harvested, the nutrient content in the harvested parts is lost from the soil system, thereby lowering the soil nutrient reserves. Non-harvested plant parts are expected to be left on the field and become part of the soil organic matter pool. As such, the nutrients in these plants are still considered as part of the soil nutrient reserve.

Yield data for the various crops from the Eurostat database have been used to establish low, high and medium yield scenarios (averages 2012-2014; Eurostat, 2016; Table 4). These yield scenarios, when combined with concentrations of the fertilizer substances in these harvested parts of the selected crops (Table 4) allow for the calculation of crop offtake, i.e. the amount of a substance that is removed from the field by harvest.

In case more up-to-date or specific data on crop substance concentration or crop yield is available, the user has the option to manually enter data in the blue fields of the input fields for Refinement options (Fig. 4). If no manual input is provided, values for the micronutrients copper, manganese and zinc, as indicated in Table 4 will be used to calculate crop offtake, depending on the crop type selected. If the FEE tool is used for assessment of another substance (selection substance 'Other'), manual input on crop substance concentration and yield is required in order to calculate crop offtake. If in this case no data is entered, crop offtake is assumed to be zero.

Table 4. European crop yield scenarios and micronutrient concentrations (Cu, Mn, Zn) for the different FOCUS crops

| FOCUS crop | European crop yield scenario (t/ha/y) ¹ | | | Crop substance concentration (g/t) ² | | |
|-----------------------------|--|------|--------|---|-----------|------|
| | Low | High | Medium | Copper | Manganese | Zinc |
| Cereals, spring | 1.9 | 6.5 | 3.5 | 11.0 | 31.0 | 24.7 |
| Cereals, winter | 1.3 | 8.0 | 4.2 | 11.0 | 21.1 | 24.0 |
| Citrus | 8.8 | 43.2 | 20.3 | 0.5 | 0.6 | 0.9 |
| Field beans | 0.6 | 5.4 | 2.5 | 13.0 | 13.0 | 38.0 |
| Grass / alfalfa | 2.0 | 27.4 | 5.3 | 6.5 | 63.0 | 39.0 |
| Hops | 0.7 | 2.0 | 1.4 | 319.0 | 84.0 | 38.0 |
| Legumes | 1.3 | 4.4 | 2.3 | 11.0 | 13.0 | 46.0 |
| Maize (grain) | 3.8 | 11.2 | 7.5 | 5.3 | 9.3 | 17.5 |
| Maize (silage) | 7.5 | 52.7 | 33.9 | 7.7 | 91.8 | 35.2 |
| Oil seed rape, spring | 1.7 | 3.0 | 1.9 | 5.0 | 33.0 | 30.0 |
| Oil seed rape, winter | 2.0 | 4.0 | 3.0 | 5.0 | 33.0 | 30.0 |
| Olives | 1.2 | 8.7 | 1.9 | no data | 2.1 | 3.1 |
| Pome / stone fruit, (early) | 2.6 | 20.8 | 8.8 | 0.7 | 1.1 | 1.7 |
| Pome / stone fruit (late) | 2.6 | 20.8 | 8.8 | 0.7 | 1.1 | 1.7 |

| FOCUS crop | European crop yield scenario (t/ha/y) ¹ | | | Crop substance concentration (g/t) ² | | |
|-----------------------------|--|-------|--------|---|-----------|------|
| | Low | High | Medium | Copper | Manganese | Zinc |
| Potatoes | 10.3 | 44.0 | 25.6 | 3.7 | 15.6 | 1.9 |
| Soybeans | 0.9 | 3.5 | 2.2 | 39.8 | 33.0 | 36.9 |
| Sugar beet | 35.9 | 90.4 | 60.7 | 0.8 | 8.0 | 3.5 |
| Sunflower | 0.7 | 2.6 | 2.3 | 9.0 | 16.0 | 46.0 |
| Tobacco | 1.4 | 2.6 | 2.0 | 21.0 | 184.0 | 69.0 |
| Vegetables, bulb | 7.7 | 29.5 | 17.3 | 1.0 | 2.2 | 4.0 |
| Vegetables, fruiting | 12.7 | 234.1 | 38.6 | 1.4 | 2.5 | 3.2 |
| Vegetables, leafy | 8.2 | 38.8 | 18.4 | 1.3 | 3.6 | 4.6 |
| Vegetables, root | 10.6 | 51.0 | 27.3 | 0.5 | 1.4 | 2.4 |
| Vines, early applications | 1.7 | 14.4 | 6.1 | 1.3 | 0.7 | 0.7 |
| Vines, late applications | 1.7 | 14.4 | 6.1 | 1.3 | 0.7 | 0.7 |
| Forest (aerial application) | 0.0 | 0.0 | 0.0 | 11.0 | 31.0 | 24.7 |

¹ Eurostat (2016)

² For a full list of references please refer to the FEE tool (sheet 'Reference list')

2.2.3. RISK MANAGEMENT MEASURES

Fertilizers, soil improvers and related products are intentionally applied to agricultural soil or crop foliage, in order to be taken up by the cultivated crops. Therefore, risk management measures (RMMs) are not relevant for the soil compartment.

The potential for emissions to surface water depends on the application technique. In all cases, operators need to comply with best application practices. For soil surface spreading of solid fertilizers (SPERC 1) and precision treatment of solid and liquid fertilizers (SPERC 2), direct emissions to aquatic systems are not relevant. For aerial application (SPERC 3) and spray application of liquid fertilizers (SPERC 4) there is a potential for direct release to surface water via drift.

For SPERC 3 and SPERC 4 it is possible, on a case-by-case basis, to select risk management measures for drift reduction. These RMMs are not included in the default release factors for the SPERCs. A drop down menu with fixed drift reduction categories is included in the tool: 50, 75 and 90% drift reduction. Selected drift reduction categories must be translated by the user into specific RMMs in correspondence with (national) requirements and product labelling. RMMs for runoff reduction (e.g. vegetative filter strips), other than refinement by crop cover on the field, are not included in the FEE tool. For more details on the RMMs for the different SPERCs is referred to the SPERC background document (Fertilizers Europe, 2017).

2.2.4. INPUT PARAMETERS E-FATE MODEL

At the bottom of the 'Input' sheet of the FEE tool a summary is provided of the parameters used for further calculations of environmental exposure, for a specific use scenario, both for the default assessment and if applicable for the refinement options introduced (blue input fields, Fig. 4). If refinement options are included, environmental fate (e-fate) calculations are being performed including these refined input parameters (Fig. 5; column "Refined assessment").

| Scenario information: SpERC 4: Outdoor use - liquid application; surface spreading, sprinkler, pivot, foliar spray, slurry | Input parameters e-fate model | | Unit |
|--|-------------------------------|--------------------|-------------------|
| | Default assessment | Refined assessment | |
| Fraction available for drift (during application) | 15,7 | 2,76 | % |
| Drift refinement, after reduction based on RMM | not considered | 0,69 | % |
| Fraction available for run-off (30 days after application) | 0,039 | 0,012 | % |
| Runoff reduction | not considered | 70 | % |
| Crop substance concentration | not considered | 10,9 | g substance/t |
| Crop yield | not considered | 6,5 | t yield/ha |
| Crop offtake | not considered | 0,070 | kg substance/ha/y |

Fig 5. Example of input parameters used for e-fate calculations.

In this specific scenario copper is applied by foliar spray (SPERC 4) on spring cereals, with a full canopy (BBCH 40-89), at a high European crop yield scenario, including 75% drift reduction. In the corresponding exposure assessment, calculations are performed using 0.69% drift ($=2.76\% \times (1-0.75)$ because of RMM), a fraction available for runoff of 0.012% ($=0.039\% \times (1-0.70)$ because of full canopy), and crop offtake of 0.070 kg/ha/y ($=0.0109 \text{ kgCu/t} \times 6.5 \text{ t/ha}$).

2.3. DEFAULT PARAMETERS AND E-FATE CALCULATIONS

2.3.1. DEFAULT PARAMETERS

For calculations of the environmental fate of a substance a number of default parameters are used in the e-fate calculations of the FEE tool. These default values are based upon the REACH R.16 guidance document (ECHA, 2016), and where needed supplemented with parameters from FOCUS Steps 1-2 model (FOCUS, 2015) or Simplebox (RIVM, 2014). A summary of all default values is presented in Table 5.

Table 5. Default parameters used for environmental exposure assessment. Reference is made to the R.16 REACH guidance document, unless otherwise specified.

| Parameters | Value | Unit | Comments |
|---------------------|-------|------|---|
| Temperature | 285 | °K | Table R.16-8 (12°C) |
| Depth soil | 0.20 | m | Table R.16-15, agricultural soil |
| Depth soil runoff | 0.02 | m | Worst-case assumption; all added fertilizer still concentrated in the top 2 cm of soil, see Chapter 2.3.2 |
| Depth surface water | 0.30 | m | FOCUS Steps 1-2 |

| Parameters | Value | Unit | Comments |
|---|----------|-------------------|--|
| Ratio field to water body | 10 | - | FOCUS Steps 1-2 |
| Density solid phase | 2500 | kg/m ³ | Table R.16-8 |
| Density water phase | 1000 | kg/m ³ | Table R.16-8 |
| Density air | 1.30 | kg/m ³ | Table R.16-8 |
| Volume fraction water in soil | 0.2 | - | Table R.16-8 |
| Volume fraction air in soil | 0.2 | - | Table R.16-8 |
| Volume fraction solids in soil | 0.6 | - | Table R.16-8 |
| Weight fraction organic carbon soil solids | 0.02 | - | Table R.16-8 |
| Concentration suspended matter in water | 15 | mg dw/L | Table R.16-8 |
| Volume fraction solids in susp. matter | 0.1 | - | Table R.16-8 |
| Volume fraction water in susp. matter | 0.9 | - | Table R.16-8 |
| Weight fraction organic carbon in susp.solid | 0.1 | - | Table R.16-8 |
| Volume fraction solids in sediment | 0.2 | - | Table R.16-8 |
| Volume fraction water in sediment | 0.8 | - | Table R.16-8 |
| Weight fraction organic carbon in sediment solids | 0.05 | - | Table R.16-8 |
| Fraction of rain water infiltrating into soil | 0.25 | - | Table R.16-18 |
| Rate of wet precipitation | 1.92E-03 | m/d | Table R.16-18 (avg.annual precipitation 700 mm/y; 2.22E-08 m/sec) |
| Fraction runoff | 0.25 | - | Simplebox Table 2; volume fraction of precipitation running off |
| Erosion | 9.51E-13 | m/s | Simplebox Table 2; erosion of soils |
| Residence time of water | 40 | d | Table R.16-18 |
| Rate of advective downward transport of soil particles | 6.34E-12 | m/d | Default R.16, pg.146 |
| Solid phase diffusion coefficient in the soil compartment | 6.37E-12 | m/d | Default R.16, pg.146 |
| Partial mass-transfer coefficient at air side of the air-soil interface | 90.72 | m/d | Table R.16-19 (1.05E-3 m/sec) |
| Density wet soil | 1700 | kg/m ³ | Default R.16, calculated Eqn R.16-1 |
| Density dry soil | 1500 | kg/m ³ | Default R.16, calculated Eqn R.16-1 |
| Water content soil | 0.13 | L/kg dw | Default, calculated from default volume fraction in soil and density of dry soil |
| Density suspended matter | 1150 | kg/m ³ | Default R.16, calculated Eqn R.16-1 |
| Density sediment | 1300 | kg/m ³ | Default R.16, calculated Eqn R.16-1 |
| Averaging time for Clocal soil | 30 | d | Default R.16, pg. 62, 127 |
| Averaging time for crop uptake | 180 | d | Default R.16, pg. 62, 127 |

2.3.2. E-FATE CALCULATIONS

For the environmental exposure assessment, the total Predicted Environmental Concentration (PEC total) is calculated as the sum of the local concentration in an environmental compartment (C local) and the relevant PEC regional.

For the micronutrients copper, manganese and zinc, information on PEC regional from the respective REACH dossiers is already incorporated into the FEE tool. Please check carefully for consistency with the most recent dossier information (see Chapter 2.4.1 for more details).

C local for soil and surface water is calculated as the time weighted average (TWA) concentration 30 days after year 1 or year 10, respectively (according to equation [R.16-43](#)). For sediment, C local is based upon the concentration in surface water and calculated as yearly TWA (according to equation [R.16-34](#)). In the next paragraphs more details on specific processes and parameters involved in the calculation of C local for the soil, surface water and sediment compartments are presented.

SOIL COMPARTMENT

In order to calculate the yearly input to the soil compartment, the application rate of a substance is corrected for removal by runoff of the fertilizer shortly after application (if applicable), removal via crop harvest, leaching to groundwater, volatilization and degradation.

Runoff

The fraction available for runoff is based upon the selected SPERC (Fig. 1); runoff is relevant for SPERC 1, SPERC 3 and SPERC 4. Refinement of the runoff fraction is possible by selection of a specific crop type (SPERC 4) and crop growth stage (all 3 SPERCs; Tables 2 and 3).

Crop Harvest

For both single and multiple applications, the local concentration in soil is also corrected for crop offtake at the end of the growing season. Crop offtake is calculated as crop substance concentration multiplied by crop yield (Chapter 2.2.3; Table 4, or based on manual input).

Leaching, volatilization and degradation

Removal from soil is expressed as a first order rate constant (k_{total} ; based on equation [R.16-44](#)), consisting of the sum of:

- Removal by volatilization (k_{volat} ; equation [R.16-45](#))
- Leaching to groundwater (k_{leach} ; equation [R.16-46](#))
- Biodegradation in soil ($k_{bio-soil}$; equation [R.16-13](#)). In case no information on biodegradation in soil is available for a substance, default values for various classes of biodegradability, depending on the partition coefficient solid-water in soil (K_{psoil}), will be used in the calculations (sheet 'Biodegradation').

For multiple applications, 'ktotal' is used to calculate removal from soil between applications (in line with calculations in FOCUS Steps 1-2) and after each year. In case of a single application per growing season, 'ktotal' is used to calculate yearly removal from top soil.

From the concentration in soil after the first year of application (according to equation R.16-48), including a factor for accumulation in soil (according to equation R.16-49), the concentration in soil after 10 years is calculated (equation R.16-50).

FRESHWATER AND SEDIMENT COMPARTMENT

For the freshwater compartment, depending on the SPERC, input can either be caused directly by spray drift during fertilizer application, or by a runoff event taking place four days after the final application (Fig. 1; in line with calculation method used in FOCUS Steps 1-2; FOCUS, 2015).

Drift

Specific drift values used for the various SPERCs and crop types are summarized in Table 2 and 3 (based upon FOCUS, 2015). Drift is only relevant for SPERC 3 and SPERC 4. For SPERC 3, drift values are always based upon the FOCUS default value for aerial application (forests). For SPERC 4 the default value is based on the FOCUS crop type 'pome/stone fruit (late)' (see SPERC background document for more details on the drift factors; Fertilizers Europe, 2017). For SPERC 4 refinement of the default drift value is possible based upon the crop type selected. In addition, for both SPERC 3 and 4, it is possible to include RMMs for drift reduction on a case-by-case basis if required (Chapter 2.2.3).

Runoff

Local scale calculations for runoff are based upon partitioning of a substance between the soil and water phase (equation R.16-7), a typical European rain rate (Table R.16-18), the default fraction of precipitation running-off (Simplebox Table 2) and a term for erosion (Simplebox Table 2). These parameters are based upon existing REACH models (EUSES, Simplebox) and were selected to represent a generic European runoff scenario (according to Simplebox equations 111 and 112). For this, the full dose of the fertilizer applied is assumed to be present in the top layer of the soil (0-2 cm) and is considered available for surface runoff. As a realistic worst-case, total rainfall of a 30-day period (based upon average daily precipitation; Table R.16-18) is assumed to fall at once, creating a runoff event four days after (the final) fertilizer application. This scenario is considered to mimic a worst-case peak release to surface water. It is assumed that the contribution of the background concentration of a substance on surface runoff is negligible compared to the applied dose in the surface (top 2 cm) of the soil profile.

For SPERC 1, crop shoots and root systems are assumed to reduce erosion and surface runoff. For SPERC 3 and SPERC 4, crop canopy interception reduces the fraction reaching the soil surface, consequently reducing the fraction available for runoff. Respective runoff reduction defaults per SPERC and per crop growth stage are based upon FOCUS interception values (Table 2 and 3).

Removal from water phase

Removal from the water phase can take place either by biodegradation or by dilution of the surface water, caused by the flow rate of the stream (residence time):

- Biodegradation (k_{bio_water_sed}); calculations are based upon REACH equation **R.16-13**. In case no information on biodegradation in the water-sediment phase is available for a substance, default values for various classes of biodegradability will be used in the calculations (sheet 'Biodegradation').
- Residence time (k_{res}); a default value of 40 days is used, in accordance with REACH R.16 guidance (**Table R.16-18**; Table 5)

Depending on the substance properties, subsequent distribution between the surface water and sediment phase takes place according to calculation methods as used in REACH R.16 guidance document (ECHA, 2016).

The FEE tool will automatically calculate the day with the highest estimated fertilizer concentration in surface water and use this value for corresponding C local calculations (after 1 and 10 year of continuous applications).

2.4. RISK ASSESSMENT

2.4.1. EXPOSURE ASSESSMENT

In the 'Output' sheet of the FEE tool, an overview of the exposure and risk assessment is presented. First, the respective exposure scenario is summarized and an overview of the emissions estimates is presented in table format and graphically (Fig. 6).

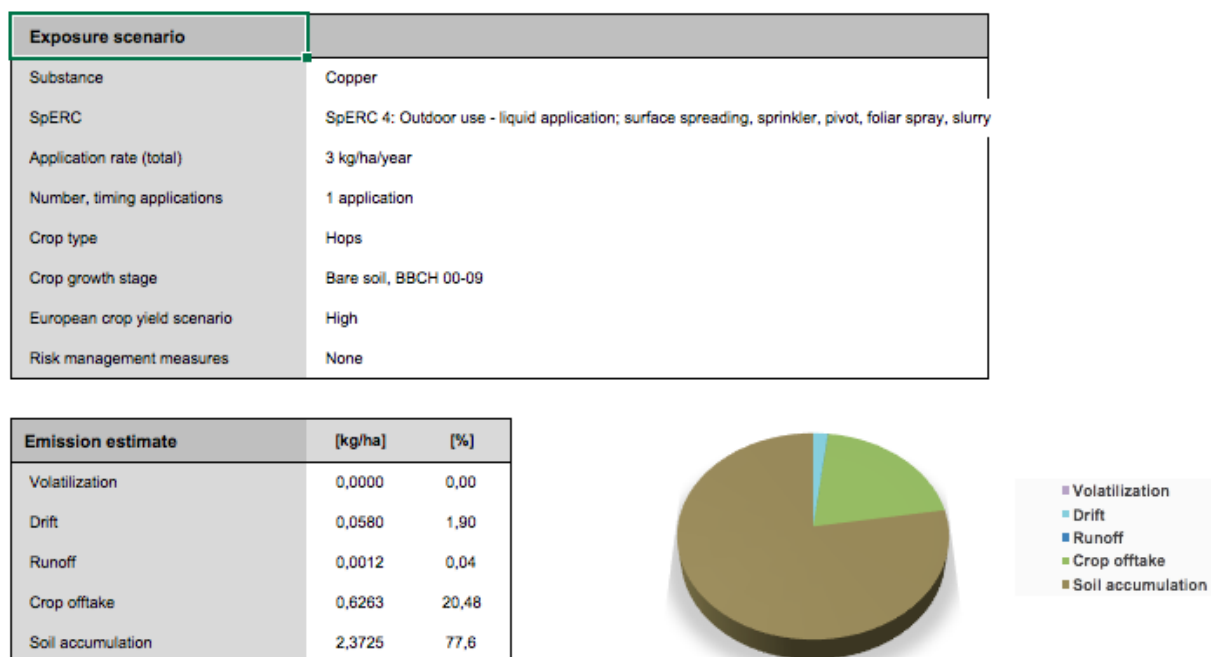


Fig. 6 Overview of the exposure scenario as specified in the 'Input' sheet of the FEE tool and corresponding emission estimates.

Local concentrations in an environmental compartment (C local, after 1 and 10 years of continuous fertilizer application at the defined rate; Chapter 2.3.2) and regional background concentrations (PEC regional) are added up to calculate the total Predicted Environmental Concentration (PEC total, after 1 and 10 years; Fig. 7)

| Environmental compartment | Exposure assessment | | | | | | Effect assessment | | Risk characterisation | |
|---------------------------|---------------------|-----------------|--------------|------------------|-------------------|----------|-------------------|----------|-----------------------|-------------|
| | C local year 1 | C local year 10 | PEC regional | PEC total year 1 | PEC total year 10 | Unit | PNEC | Unit | RCR year 1 | RCR year 10 |
| Soil (agricultural) | 1,00 | 10,0 | 14,0 | 15,0 | 24,0 | mg/kg dw | 65,0 | mg/kg dw | 0,23 | 0,37 |
| Freshwater (dissolved) | 1,8 | 1,8 | 2,9 | 4,7 | 4,7 | µg/L | 7,8 | µg/L | 0,61 | 0,61 |
| Sediment | 1,9 | 1,9 | 67,5 | 69,4 | 69,4 | mg/kg | 87,0 | mg/kg | 0,80 | 0,80 |
| Groundwater | | | | 0,0080 | 0,0128 | mg/L | | | | |

Fig. 7 Summary of the exposure assessment, effect assessment and risk characterisation as presented in the 'Output' sheet of the FEE tool.

For the micronutrients copper, manganese and zinc, values for PEC regional are already included in the FEE tool (based upon information in the respective REACH dossiers) and automatically included upon selection of the substance in the 'Input' sheet. When natural background concentrations are included in the assessment (total risk approach), as is the case for example for Cu, the PEC regional value in soil should be revised in order to reflect that fertilizers are only to be used in deficient soils. An adapted PEC regional value for Cu is used in the FEE tool automatically. For details on the selected PEC regional values, is referred to the respective REACH dossiers. In case the tool is used for assessment of other substances, this data needs to be added manually to the 'Input' sheet in the blue fields of the 'Substance properties' table.

2.4.2. EFFECT ASSESSMENT

For risk characterisation, PEC totals are compared to Predicted No Effect Concentrations (PNEC values; Fig. 7), in order to assess if a specific use scenario can be considered safe. As for the PEC regionals, for copper, manganese and zinc, PNEC values have been included in the FEE tool and will be automatically used in the risk assessment of the respective substances.

For Manganese a revised PNEC_{soil} value is incorporated into the FEE tool: PNEC_{soil} = 12.4 mg/kg dw, i.e. 10% of the 10th percentile of aqua regia soluble Mn concentrations in European arable soils (based upon GEMAS database; Reimann et al., 2014). The PNEC_{soil} reported in the REACH dossier for manganese (3.4 mg Mn/kg) is considered over-conservative and not appropriate for fertilizer applications in Mn deficient soils.

For details on the other PNEC values, is referred to the respective REACH dossiers. Please carefully check for consistency with the most recent information on the ECHA dissemination website (<https://echa.europa.eu/web/guest/information-on-chemicals>). In case the tool is used for assessment of other substances, this data needs to be added manually to the 'Input' sheet in the blue fields of the 'Substance properties' table, in order to perform a full risk assessment.

2.4.3. RISK CHARACTERISATION

The ultimate goal of the FEE tool is to assess under which conditions fertilizer substances can be used safely. Depending on the input parameters added in the 'Input' sheet of the tool, the estimated PEC will be compared to the relevant PNEC for each environmental compartment, and a risk characterisation ratio (RCR, after 1 and 10 year) will be calculated. If the RCR is below one (fields in green; Fig. 7) the respective use scenario is considered safe for the environment.

To aid the user in the environmental exposure assessment of specific fertilizer use scenarios, the FEE tool automatically calculates the 'Maximum estimated safe application rate' (as total yearly application rate, after 1 and 10 years; Fig. 8). This safe application rate is based upon a selected target RCR (default RCR = 0.90; value can be adapted by user), and takes into account the most sensitive environmental compartment for a specific use scenario.

| Maximum safe application rate calculation | | |
|--|------------|------------|
| Most sensitive environmental compartment year 1 | freshwater | |
| Most sensitive environmental compartment year 10 | soil | |
| Target RCR | 0,90 | |
| Estimated max application rate year 1 | 13,62 | kg/ha/year |
| Estimated max application rate year 10 | 3,36 | kg/ha/year |

Fig. 8 Maximum safe application rate calculated for a specific use scenario.

2.4.4. EXTREME FERTILIZER APPLICATION RATES

In case of extreme fertilizer application rates, used sporadically to boost soil fertility and crop performance (e.g. applied once every 5 or 10 years), it is important to calculate the impact of these extreme applications correctly. In the FEE tool it is not possible to do this automatically. Instead two separate calculation runs need to be performed; one to calculate peak exposure in surface water, sediment and soil and one run to calculate accumulation based on an average application rate over 10 years. In this way, both peak exposure and accumulation potential can be assessed, without being over-conservative.

PEC surface water concentrations will decrease over time caused by degradation, renewal and refreshing of the water system by natural flow rate of the water body. Therefore, the surface water compartment is very sensitive to peak emissions and for PEC calculations for surface water and sediment, a maximum/extreme yearly rate generally results in the highest risk characterisation ratios (RCR 1 year). For PEC soil calculations, gradual accumulation of the substance in soil over time is the most important process (except for highly degradable organic substances). Therefore, an average yearly application rate over 10 years (instead of 10 years of extreme applications, which is not a standard agricultural practice) generally results in the largest RCR for soil.

Example: Copper is applied once every 5 years at an extreme application rate of 10 kg/ha. For peak exposure assessment of surface water, sediment and soil, first the FEE tool is used to calculate an application rate of **10 kg/ha** (input in field 'Total annual fertilizer use rate') and results for the RCR soil 1 year, RCR surface water 1 year and RCR sediment 1 year are taken into account. Next, accumulation is assessed by performing the same model run, but now entering an application rate of **2 kg/ha** (2*10 kg in 10 years, equals an average of 2 kg per year; input in the field 'Total annual fertilizer use rate'). In this case the RCR 10 years for soil, freshwater and sediment is the relevant result. Only if all RCRs of the two model runs are below 1, the use can be considered safe.

2.4.5. COMBINATION OF DIFFERENT APPLICATION TECHNIQUES

In case a fertilizer is applied several times during one growing season using a combination of different application techniques belonging to different SPERCs, combined risk characterisation ratios for all application techniques together cannot be calculated automatically using the FEE tool. Instead multiple separate calculation runs need to be performed; one run for each application technique (or SPERC) used. From each run predicted concentrations in the environmental compartments (C local year 1 and C local year 10) can be retrieved and combined with the respective background concentration in order to manually calculate a PEC local for each compartment. This calculated PEC total can be compared to the respective PNEC, in order to derive relevant RCR's.

Example: Zinc is applied several times during the growing season. First application is by SPERC 2 (2 kg/ha), followed by multiple applications of SPERC 4 (0,5 kg/ha; 2 applications with a 14 days interval). In this case 2 runs of the FEE tool are needed.

Run 1: Single application of 2 kg/ha of SPERC 2. This will result in a C local year 1, C local year 10 and a PEC regional (values to be found in the 'Output' sheet of the tool). For example, this will return a C local soil year 1 of 0.67 mg/kg and a PEC regional of 41.3 mg/kg.

Run 2: Multiple applications of SPERC 4. In this case a total annual fertilizer use rate of 1 kg/ha, with 2 applications, 14 days time between applications. This will result in a second C local year 1 and C local year 10. PEC regional will be identical to that of Run 1. In this example, the resulting C local soil year 1 will be 0.33 mg/kg.

In order to calculate the PEC total year 1 for the soil compartment, C local year 1 of Run 1 needs to be added to C local year 1 of Run 2 and PEC regional; $PEC\ soil\ year\ 1 = 0.67 + 0.33 + 41.3 = 42.3\ mg/kg$. Compared to a PNEC soil for zinc of 107.0 mg/kg, this would lead to an RCR soil year 1 of 0.40 (safe use).

2.4.6. SECONDARY POISONING AND MAN VIA ENVIRONMENT

The focus of the FEE tool is on the assessment of direct toxicity. Secondary poisoning to mammals and birds through the food chain is not a critical exposure pathway for essential elements such as copper, manganese and zinc, since internal concentrations of these substances can be actively regulated (homeostasis) by organisms.

Assessment of exposure of man via the environment is not included in the FEE tool, since this is for most metal compounds based upon monitoring data rather than modelled data. Nevertheless, PECs calculated using the FEE tool can be used as basis for further assessment, in combination with other data from the respective REACH dossiers.

3. REFERENCES

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