National Institute for Public Health
and the Environment
Ministry of Health, Welfare and Sport

Release note to SimpleTreat version 4.1.0

National Institute for Public Health and the Environment (RIVM).

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Contents

1. Bugs fixed

1.1 Degradation in aerator

Degradation rates selected from Method 1 (tab Biodegradation) are now applied to box 5 of the model only. Box 5 is the aqueous phase of the aerator [1]. In previous ST versions, the rate constants selected in Method 1 were erroneously applied to box 5 and box 6.

1.2 Temperature field used with custom biodegradation rate constants

In previous ST versions, the temperature that was indicatively shown in the greyed out temperature field when selecting a standard biodegradation rate constant from 'Method 1' (tab Biodegradation) was used (in some cases) for temperature correction of the selected rate constant. E.g. when a temperature and rate constant (not a temperature alone) was entered in Method 2 and after a

calculation, Method 1 was selected, the temperature from the previous Method 2 calculation, although shown as greyed out, was applied to the selected Method 1 rate constant.

In this update, the standard rate constants in Method 1 are no longer coupled to a temperature, see also section 2.1. The standard rate constants now apply 'as is', i.e. they are not coupled to any temperature. The option 'Apply custom biodegradation rate constant' can be used to temperature correct any rate constant in Method 1.

1.3 Temperature correction of Henry's law constant

In previous versions, the temperature correction for the user entered Henry's law constant (*H*) was performed with a molar enthalpy of 10 kJ mol^{-1}. This is corrected. The molar enthalpy now used is $H_{0\ vapour}$-$H_{0\ solut}$ (see equation 3), amounting to 50-10 = 40 kJ mol^{-1}.

1.4 Inadvertent retaining of degradation rate constants

In some instances, biodegradation rate constants entered under Method 1, 'Custom biodegradation rate constant', or Method 2 or 3 were retained when they should have been reset to the default value that was shown in the greyed out field. This could occur e.g. upon switching between Methods or when toggling between SimpleTreat 3.1 and 4.1 mode.

2. Other changes

2.1 Temperature field for standardised biodeg rate constants

The five standardised biodegradation rate constants that can be selected under 'Method 1' from the pull down menu (tab Biodegradation) no longer show a temperature in the temperature field.

In previous ST versions this field which was greyed out, and a temperature was indicatively shown, but it was not possible to enter or change a temperature.

2.2 Access database omitted

Earlier versions of ST made use of a Microsoft™ Access database to temporarily store data (e.g. when performing an Export of results to MS Excel). In recent years this led to error messages of the type: 'Problem initializing application, make sure Microsoft's Data Access Components (MDAC) are installed on your PC' and 'The Microsoft.ACE.OLEDB.xx.0' provider is not registered on the local machine'. By circumventing the use of the temporary MS Access database, the MDAC file is no longer needed and the error message does no longer occur.

2.3 Surplus sludge

The parameter Surplus sludge (SU, equation 3 in Struijs, 2014 [1]), has been added to the SimpleTreat export. When results of a ST run are exported (Menu bar, Export) to pdf or a spreadsheet, the new section **Model parameters** contains the calculated value of SU in kg_{dwt} PE^{-1} d^{-1}. SU can not be altered by the user directly. It is dependent on various model parameters, all of which can in principle altered by the user (see Struijs [1] for details).

EU guidance documents for the REACH [2] and biocides [3] frameworks display a default value for Surplus sludge in the calculation of SLUDGERATE. The latter parameter is used in these guidance documents to calculate C_{sludge}, which in turn determines the concentration of a chemical spread onto soil with sewage sludge in their exposure models. However, if one of the model parameters that influences SU is changed, SU changes as well. The applicable value for SU can now be obtained from the export.

An alternative is to retrieve C_{sludge} directly from the Concentrations tab in the model.

3. Temperature correction of input parameters in SimpleTreat standalone software

With the release of SimpleTreat version 4.0.8, the possibility of temperature correction of the chemical substance parameters vapour pressure (V_p), water solubility (S), Henry's law constant (H) and biodegradation rate constants (k_{biodeg}) was implemented. Since the SimpleTreat 4.0.8 update was performed after the release of RIVM report 601353005 [1] and UBA report 13/2015 [4], the underlying equations and default values used in these temperature corrections had not been published. This release note fills this gap and describes how temperature correction is implemented in SimpleTreat version 4.1.

Equations to correct *V*p, *S* and *H* are provided in ECHAs guidance on the Biocidal Products Regulation (BPR), Volume IV, Parts B + C [3] and are repeated below.

Vapour pressure

$$Vp_{Tenv} = Vp_{Ttest} \cdot e^{\frac{Ho_{vapour}}{R}\cdot\left(\frac{1}{T_{test}}-\frac{1}{T_{env}}\right)} \quad (1)$$

Water solubility

$$S_{Tenv} = S_{Ttest} \cdot e^{\frac{Ho_{solut}}{R}\cdot\left(\frac{1}{T_{test}}-\frac{1}{T_{env}}\right)} \quad (2)$$

Henry's law constant

$$H_{Tenv} = H_{Ttest} \cdot e^{\frac{H_{0\ vapour}-H_{0\ solut}}{R}\cdot\left(\frac{1}{T_{test}}-\frac{1}{T_{env}}\right)} \quad (3)$$

Biodegradation rate constants

$$k_{biodeg\_Tenv} = k_{biodeg\_Ttest} \cdot e^{\frac{E_a}{R}\cdot\left(\frac{1}{T_{test}}-\frac{1}{T_{env}}\right)} \quad (4)$$

Explanation of symbols

Symbol	Description	Unit	Value
E_a	molar activation energy for biodegradation	[kJ mol^{-1}]	65.4
$H_{0\ solut}$	molar enthalpy of dissolution	[kJ mol^{-1}]	10
$H_{0\ vapour}$	molar enthalpy of vaporisation	[kJ mol^{-1}]	50
k_{biodeg_Tenv}	biodegradation rate constant at the environmental compartment temperature	[d^{-1}]	
k_{biodeg_Ttest}	biodegradation rate constant at the experimental temperature	[d^{-1}]	
R	gas constant	[Pa m^3 mol^{-1} K^{-1}]	8.314472
S_{Tenv}	water solubility at the environmental compartment temperature	[mg L^{-1}]	

Symbol	Description	Unit	Value
S_{Ttest}	water solubility at the experimental temperature	[mg L^{-1}]	
T_{env}	temperature of the environmental compartment	[K]	15
T_{test}	temperature of the experiment in which the measured variable was determined (V_p, S, H, k_{biodeg})	[K]	
Vp_{Tenv}	vapour pressure at the environmental compartment temperature	[Pa]	
Vp_{Ttest}	vapour pressure at the experimental temperature	[Pa]	

Note 1.

The value for the gas constant R used in SimpleTreat deviates from the value currently reported in ECHAs BPR guidance. The value used in SimpleTreat is 8.314472 [5]. It has a higher number of significant digits than the value presented in ECHAs BPR guidance [3].

Note 2.

The value used for the molar activation energy for biodegradation, E_a (65.4 kJ mol^{-1}) in SimpleTreat corresponds with the value derived within the European regulatory framework for plant protection products (EFSA) [6], which is also used in the European biocides framework for groundwater modelling purposes ([7], p. 13, entry nr. 23). Although the use of the value for E_a in the BPR framework has not yet been implemented in the overall guidance document [3], SimpleTreat does make use of this value in temperature correction of biodegradation rate constants.

Note 3.

Biodegradation rate constants presented under Method 1 are estimated from OECD/EU standardized biodegradability tests OECD 301, 302 and 310. In ST v 4.1, no temperature is assigned to these rate constants. For users within the European biocides regulatory framework, this means that these rate constants are valid at the default temperature of the STP [1] of 15°C (288.15 K). This agreement is listed as TAB ENV entry nr.9 in the EU BPR framework [7].

The user can not alter the value, nor the temperature of the standardized rate constants shown under Method 1. In case the user wants to apply temperature correction in Method 1, either to one of the standardized degradation rates or to any other rate constant that the user has available that should be used in Method 1, this is possible via the option 'Apply custom biodegradation rate constant' in Method 1.

4. References

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