Parameter estimation for outdoor water-sediment studies by B. Gottesbüren

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- laboratory vs. outdoor water/sediment system
- experimental setup and conditions
- parameter estimation process
- use of the parameters in TOXSWA and FOCUSsw calculator (Dec. 2000)

Comparison of laboratory vs. outdoor water sediment study

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Conditions	Laboratory	Outdoor
radiolabel?	yes	yes
Dimensions	5 cm water	20 –30 cm water 2 cm sediment
Temperature	Constant @ 20°C	natural variation
Irradiation	dark	global radiation

Schematic details of the experimental setup for the water-sediment study under outdoor conditions

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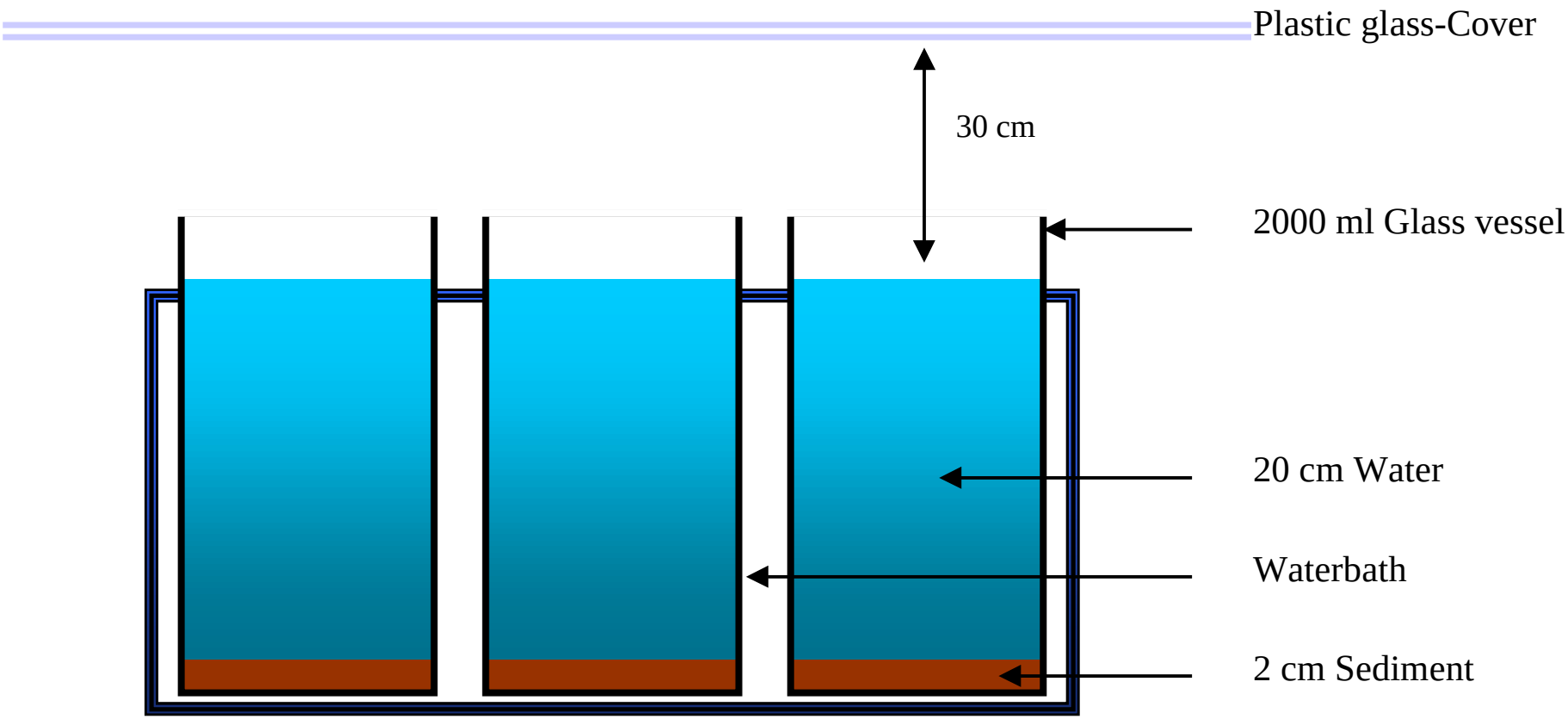

Water temperature and Global Radiation in the outdoor water-sediment study

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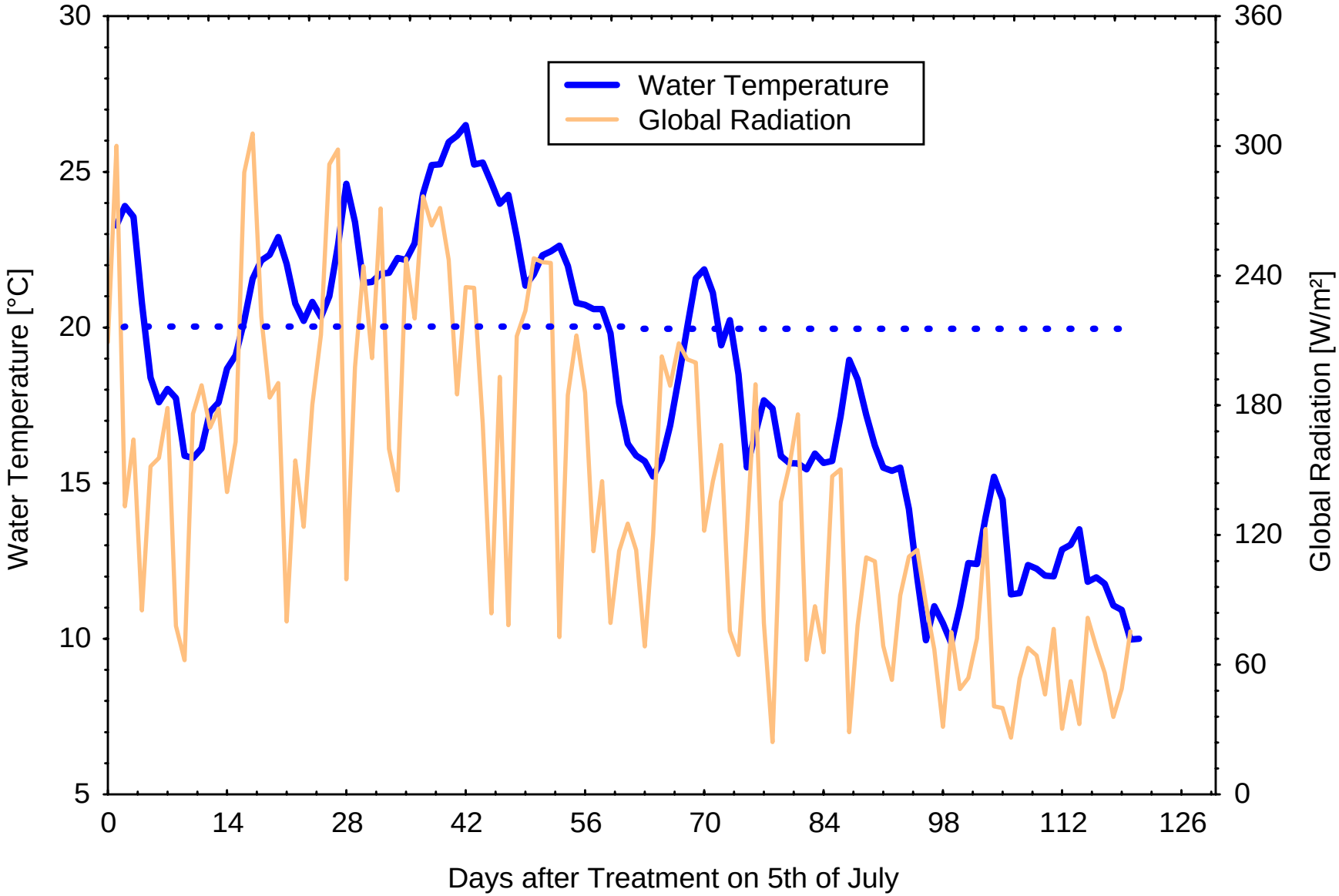

Global Radiation in Summer in Europe (July-September)

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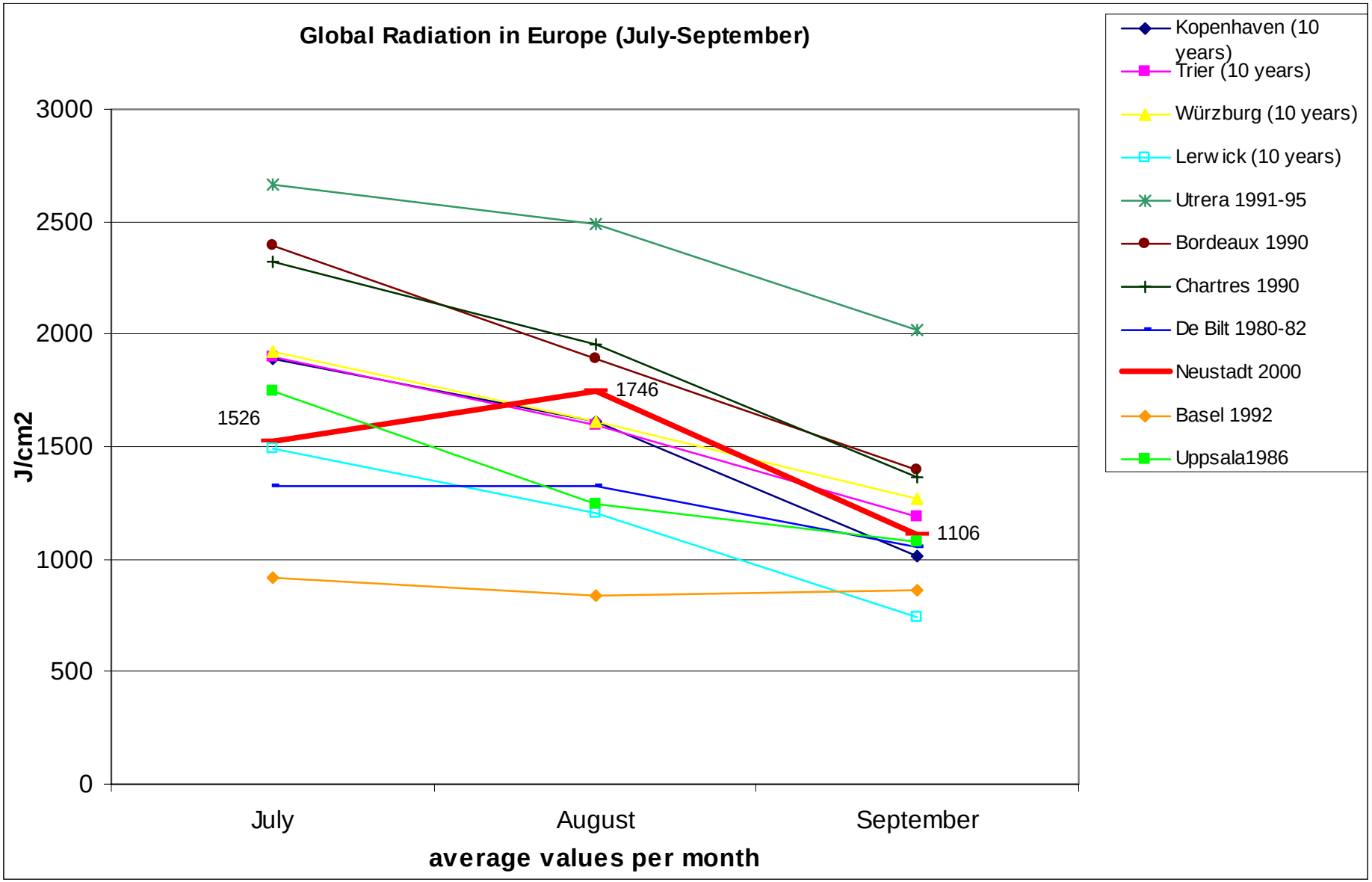

Standardisation of degradation rate constants

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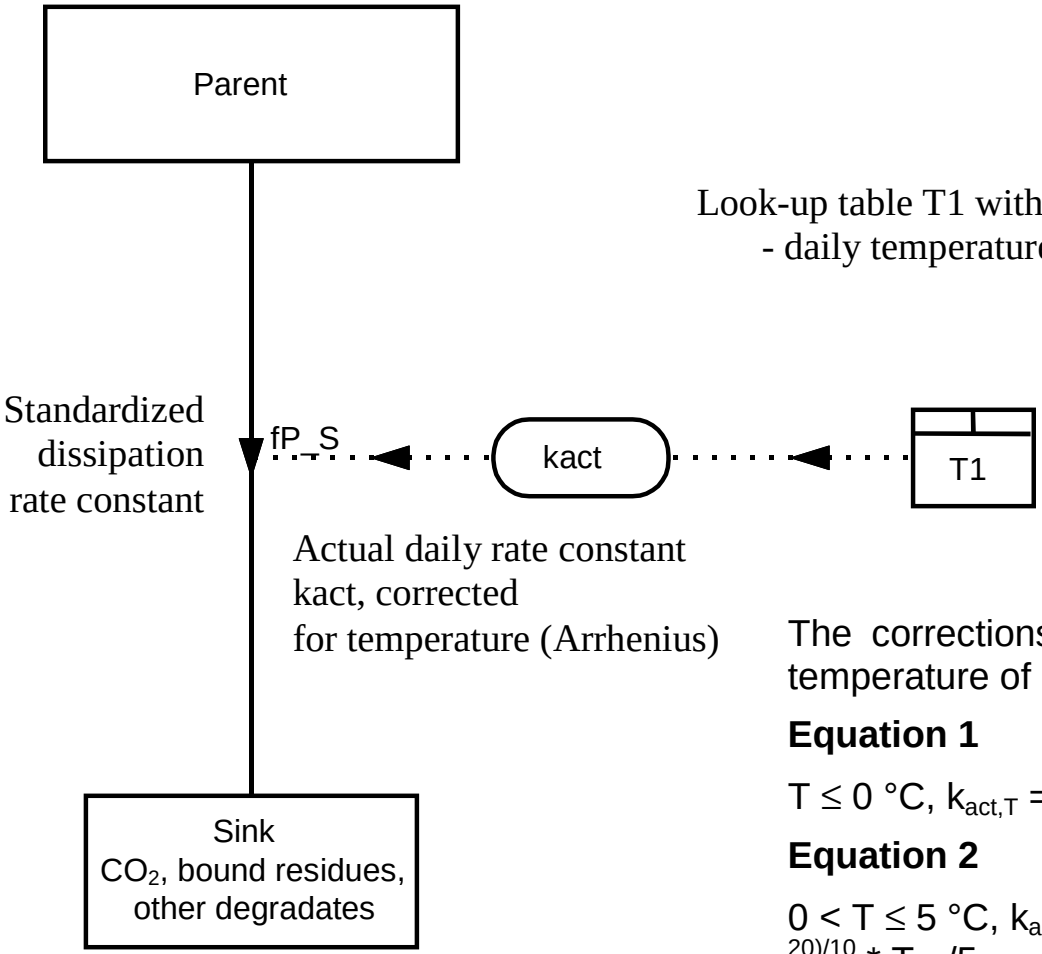

The corrections from the actual temperature T to the referen temperature of 20 °C were made with Equation 1 to Equation 3

Equation 1

$T \leq 0$ °C, $k_{act,T} = 0$ (no degradation)

Equation 2

$0 < T \leq 5$ °C, $k_{act,T} = k_{standardized} * 2.2^{(5-20)/10} * T_{act}/5$ (linear relationship)

Equation 3

$T > 5$ °C, $k_{act,T} = k_{standardized} * 2.2^{(Tact-20)/10}$ (Q_{10} equation, based on Arrhenius, with default value of Q_{10} of 2.2)

Comparison of aquatic dissipation of of PPP1 in lab. vs. outdoor water/sediment systems

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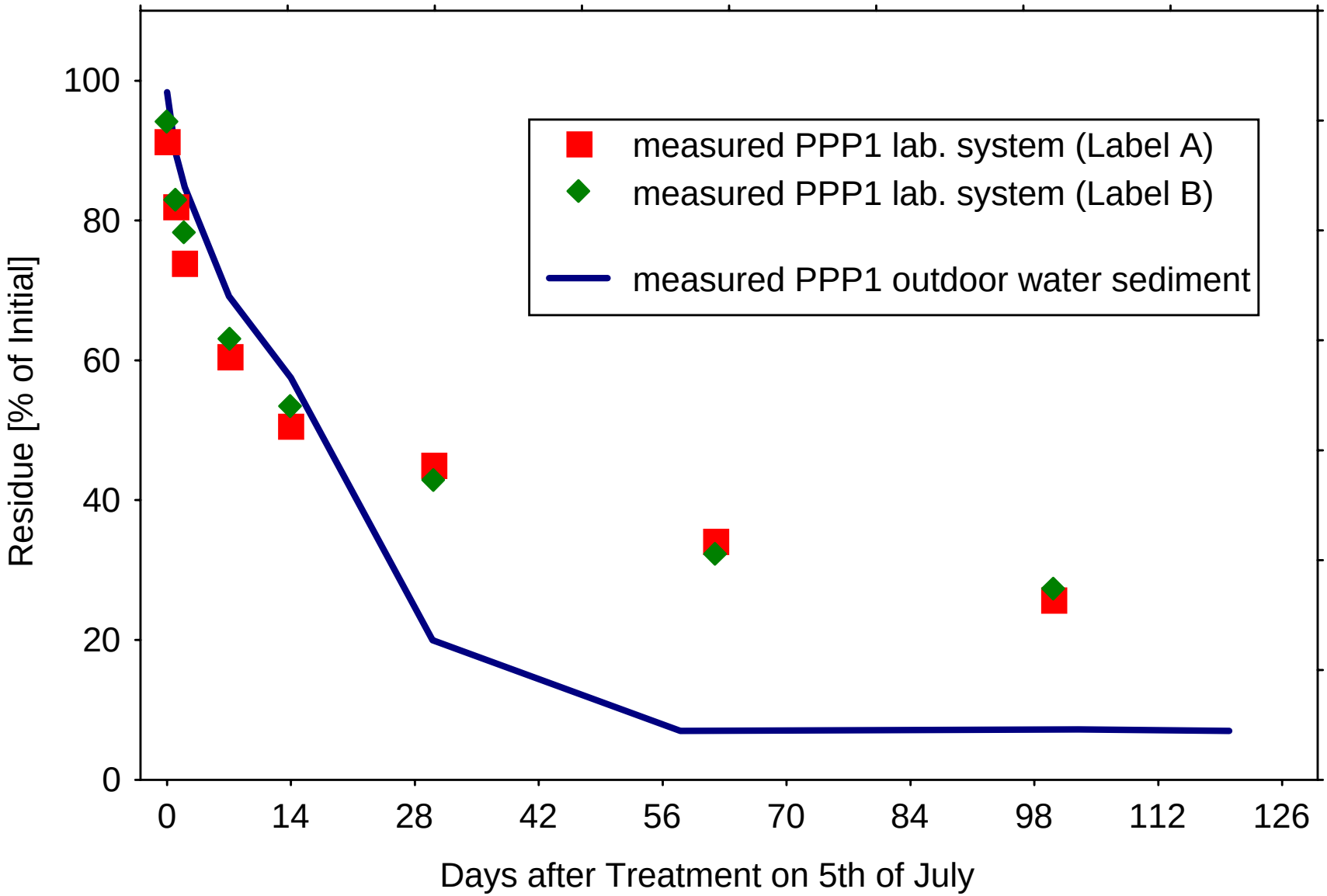

PPP2 in water and sediment phase and temperature fluctuations

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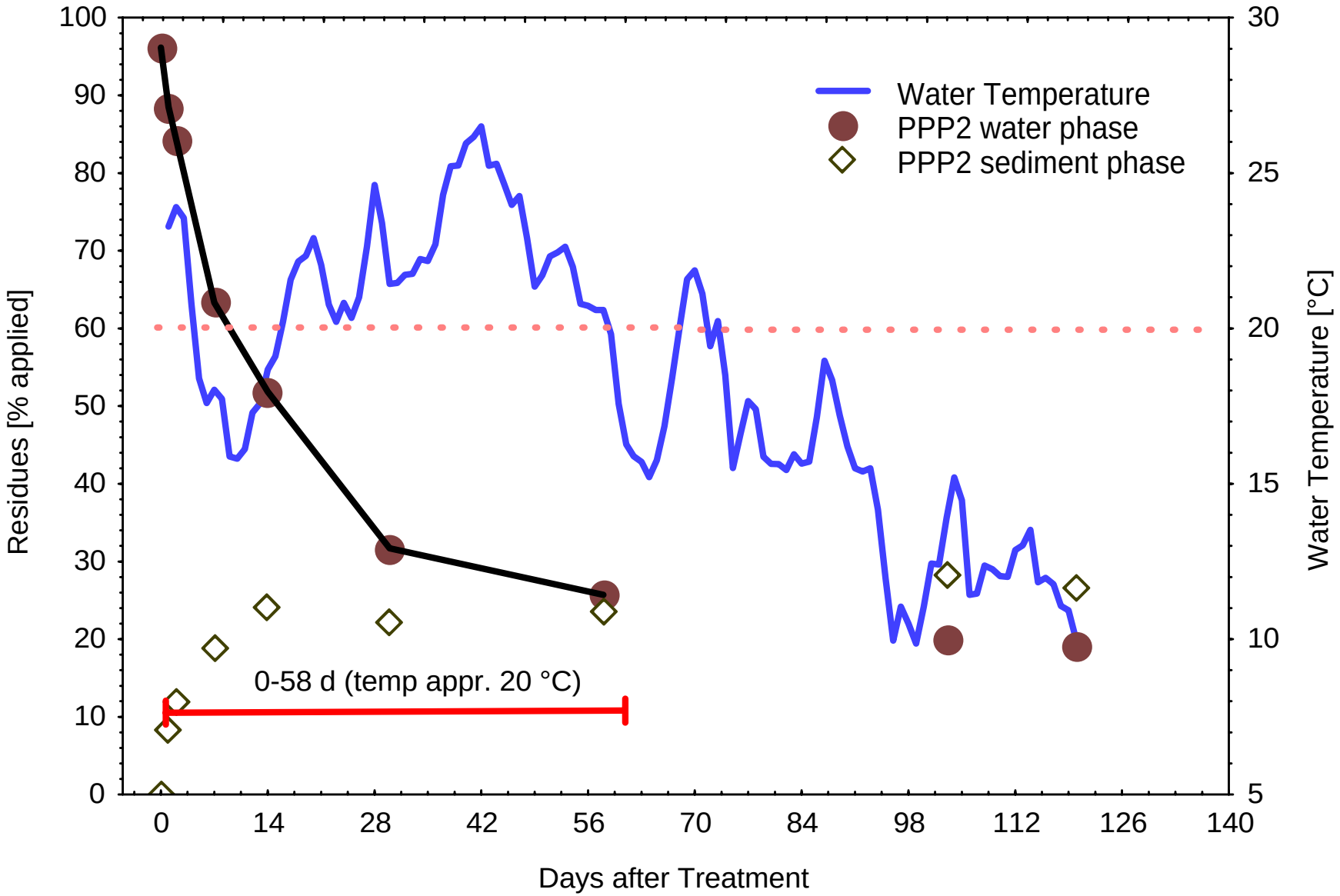

Measured, fitted and simulated concentrations of PPP2 in the water phase

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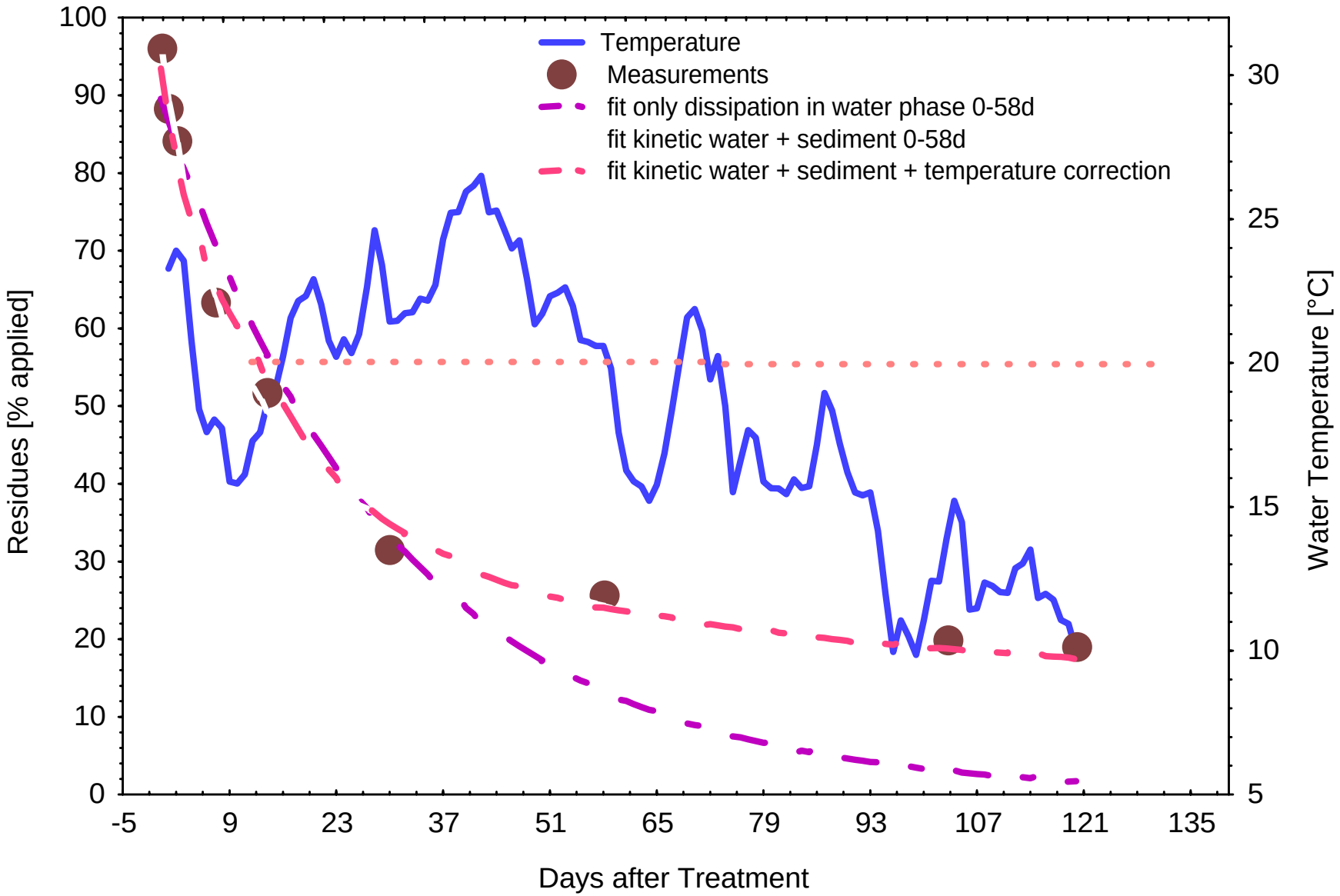

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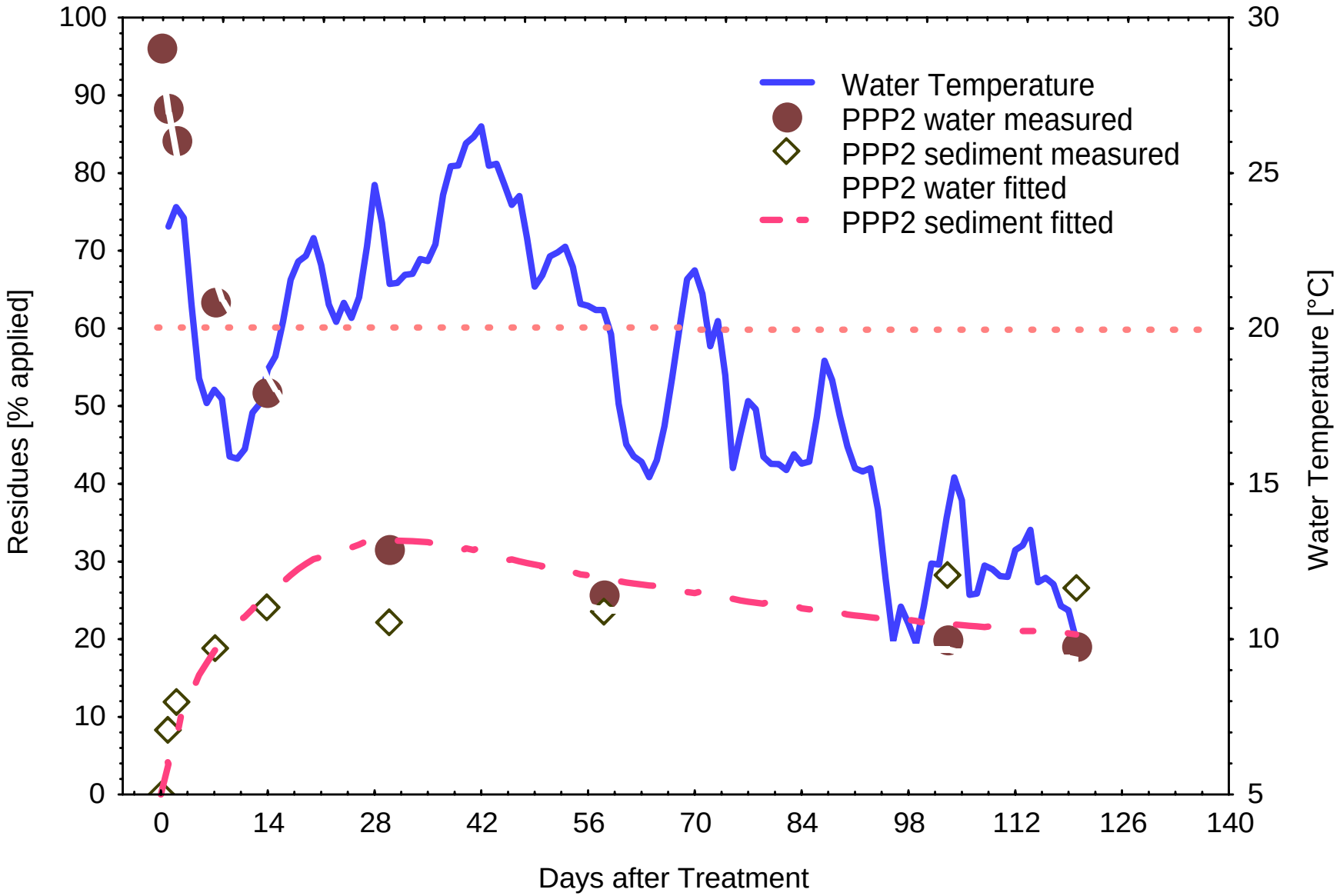

Comparison of aquatic dissipation of of PPP2 in lab. vs. outdoor water/sediment systems

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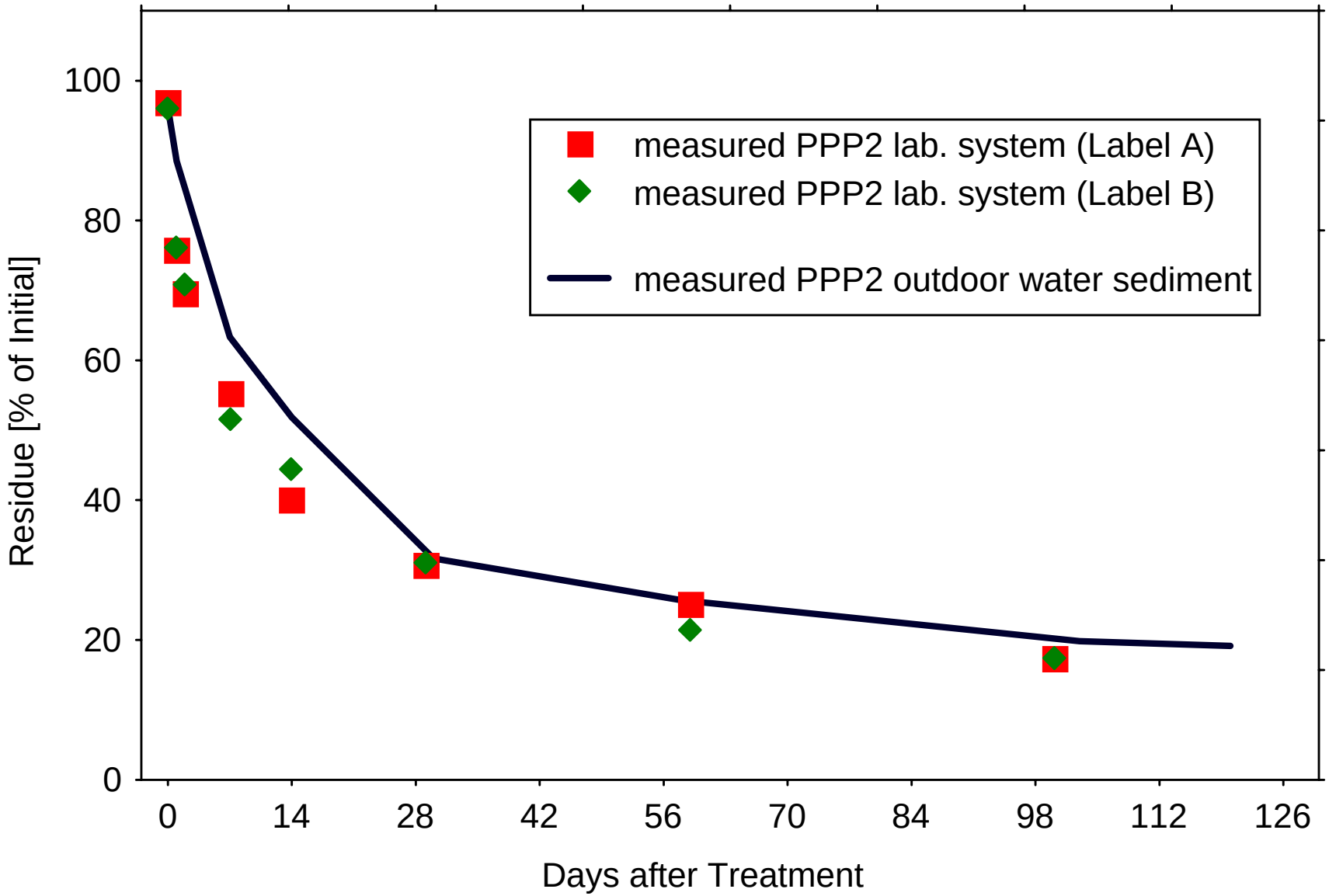

Use of the parameters in TOXSWA and in FOCUSsw calculator (Dec. 2000)

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- static water body !
- DT50 in water and in sediment from outdoor water/sed. study
- KOM from soil adsorption studies
- water temp. set constant @ 20 °C
- only drift as entry route

Measured, fitted and simulated concentrations of PPP2 in the water phase

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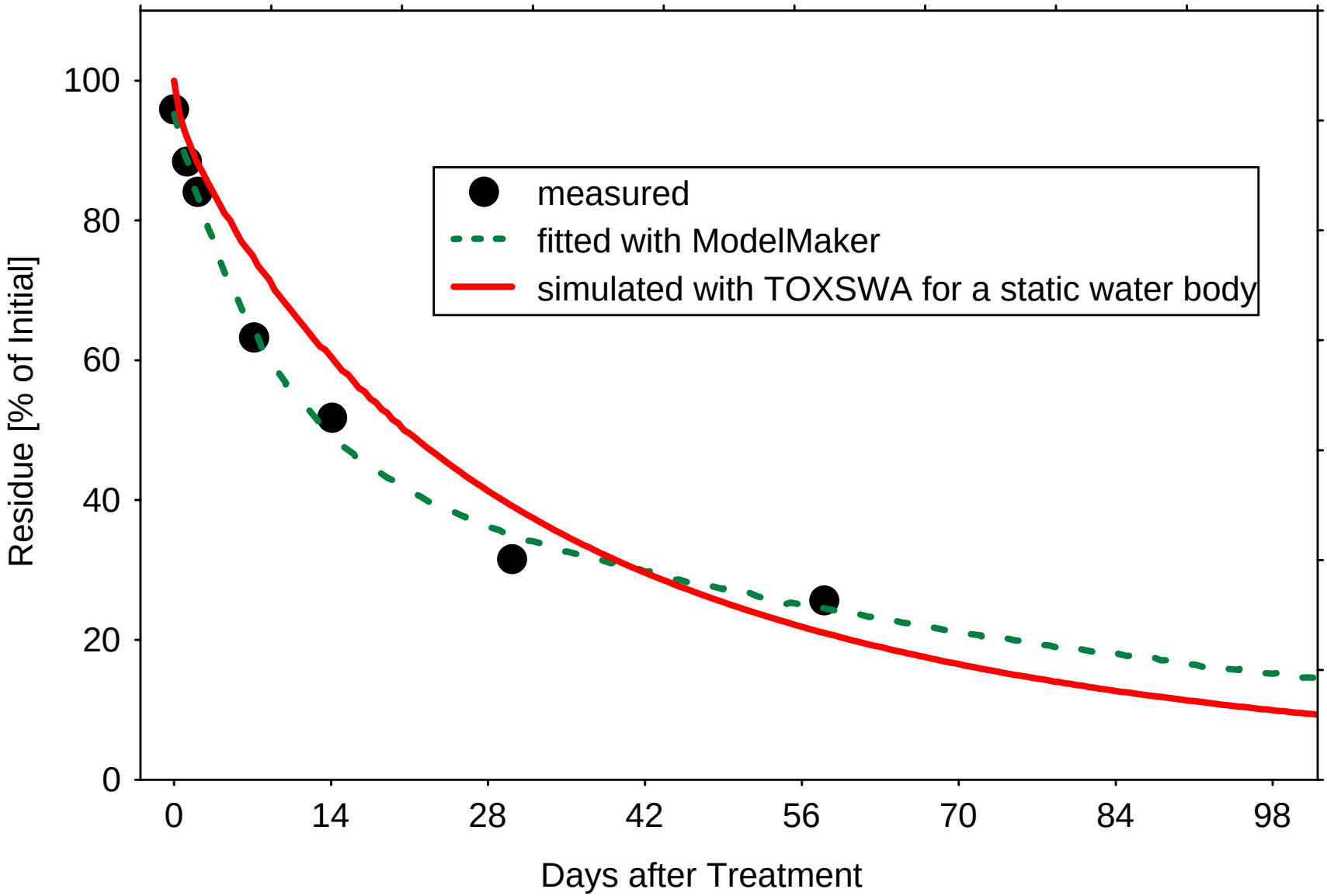

Measured, fitted and simulated concentrations of PPP0 in the water phase

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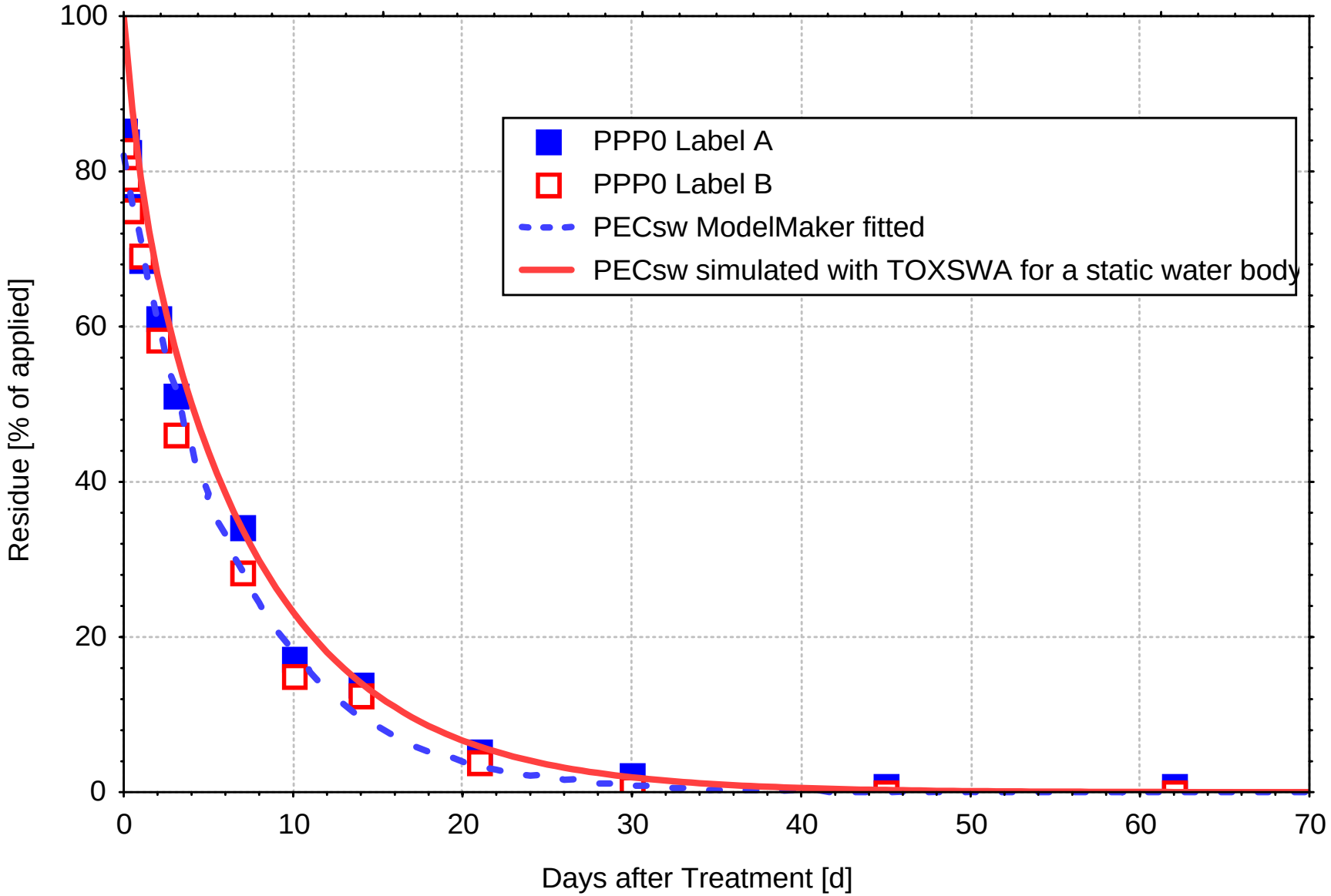

Measured, fitted and simulated concentrations of PPP1 in the water phase

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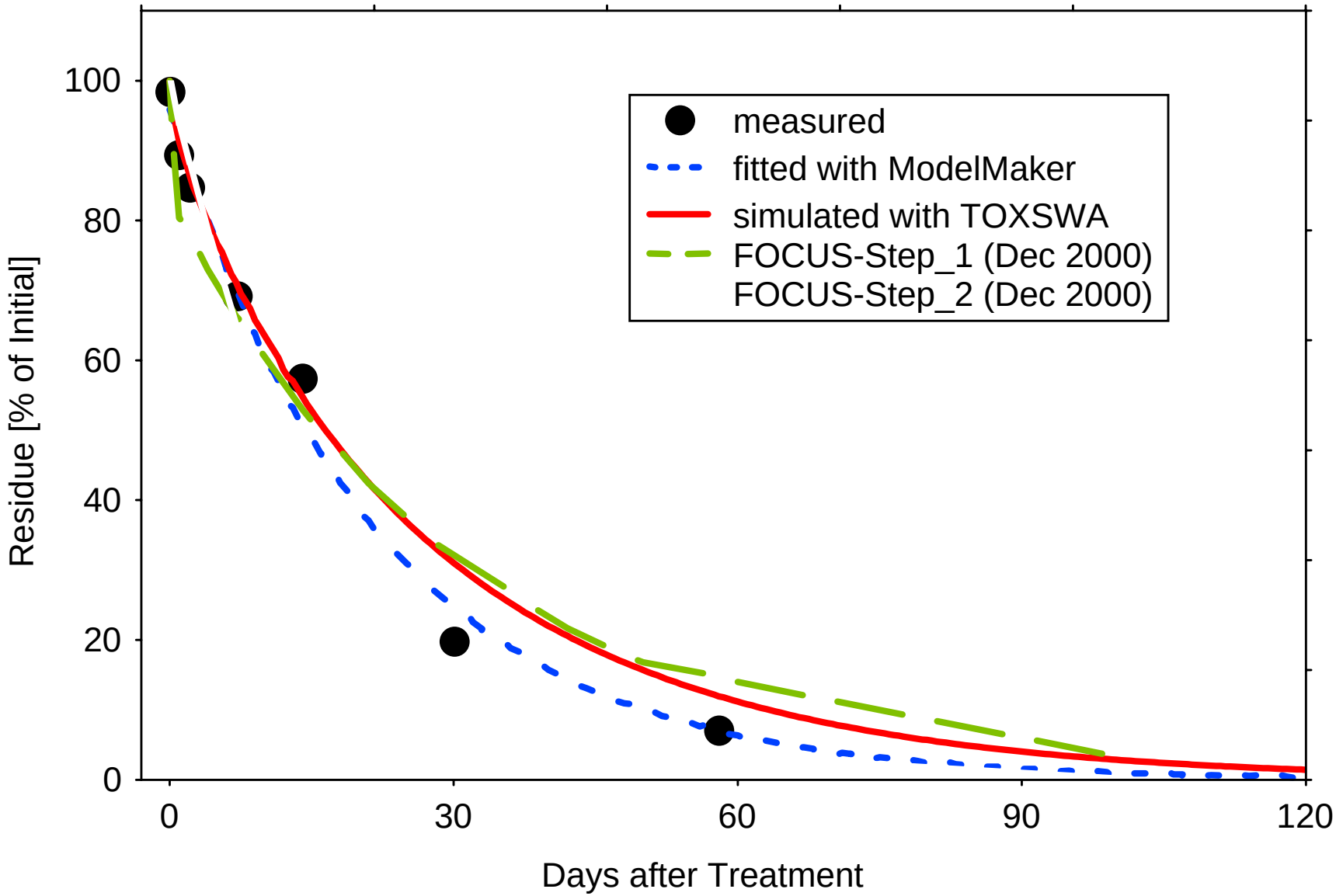

Conclusions

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- Outdoor water/sediment studies
are more realistic than laboratory studies

- Suitable as a higher tiered study type

- Parameters can be successfully estimated

- Preliminary experiences for Use with TOXSWA
and with FOCUSsw calculator are promising