Supporting Information to:

Modelling Metaldehyde in Catchments: A River Thames Case-Study

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1. The INCA-Contaminants Model

Figure SI1 illustrated the structure of the INCA-contaminants land phase model. In the land phase model, the soil has been divided into two layers which are conceptualized as a superficial organic layer and an underlying mineral layer. Each layer contains soil air and soil water (which includes the fraction of dissolved organic carbon, DOC, and soil organic carbon, SOC). The relative volumes of soil air and soil water are dynamically determined by the inputs of SMD. In addition, the SOC is divided into two pools representing easily and potentially accessible fractions to allow a better simulation for contaminants interaction with the solid organic phase and to allow for different breakdown rates in soils in relationship to the contaminant pool availability to degrading microorganisms. Within the soil, the main transport processes represented in the model include: partitioning among sub-phases of the soil layers; gaseous diffusion across the atmosphere and the upper soil layer, diffusion across the upper and lower soil layer in the soil water and soil air; bioturbation; and vertical advection (leaching) from upper to lower soil layer. The outputs of contaminants from the soil layers include surface and diffuse runoff from the upper layer and diffuse runoff from the lower layer and the degradation of contaminants.[1]

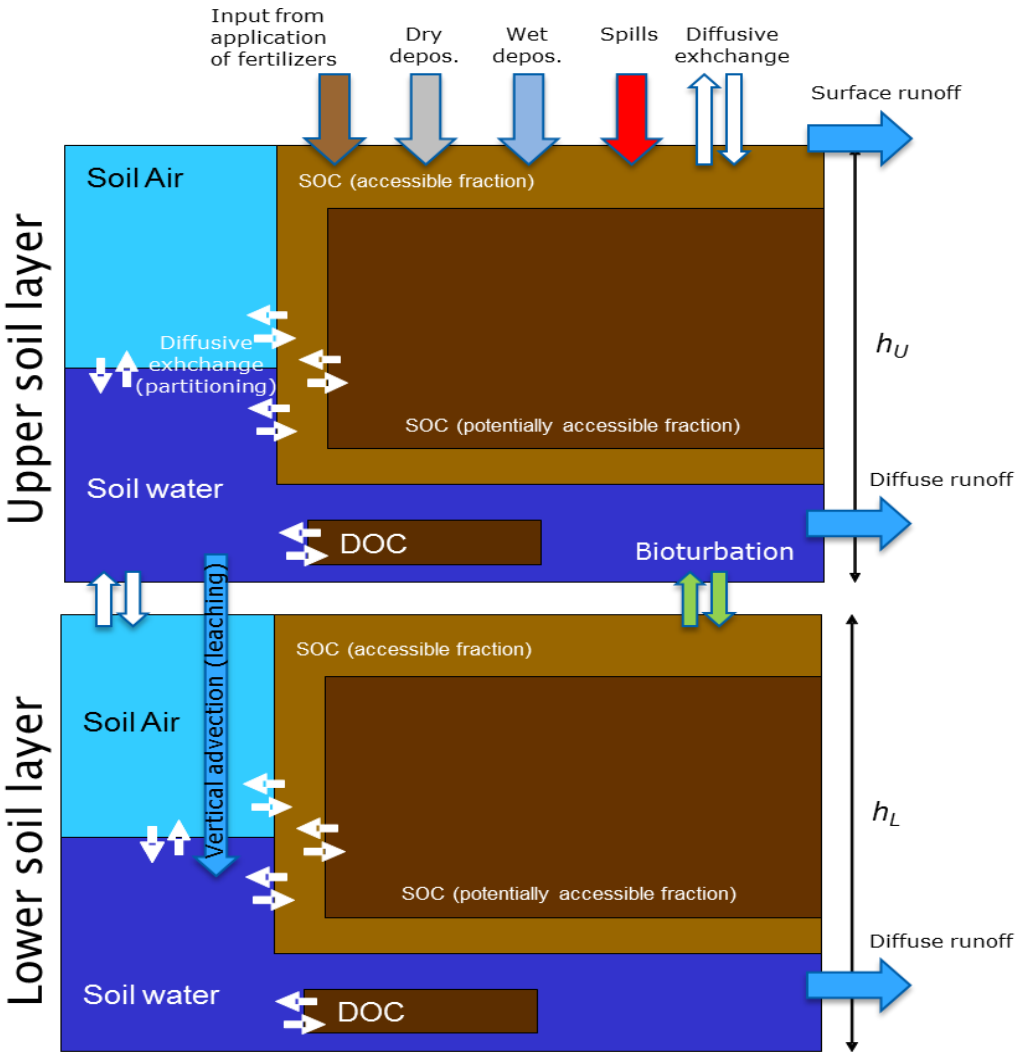

Figure SI1. Structure of the soil compartment, adapted from Nizzetto et al. (2016) [1, 2]. The degradation process (not depicted in the figure) occurs in any of the soil sub-compartments with independent user-definable rates.

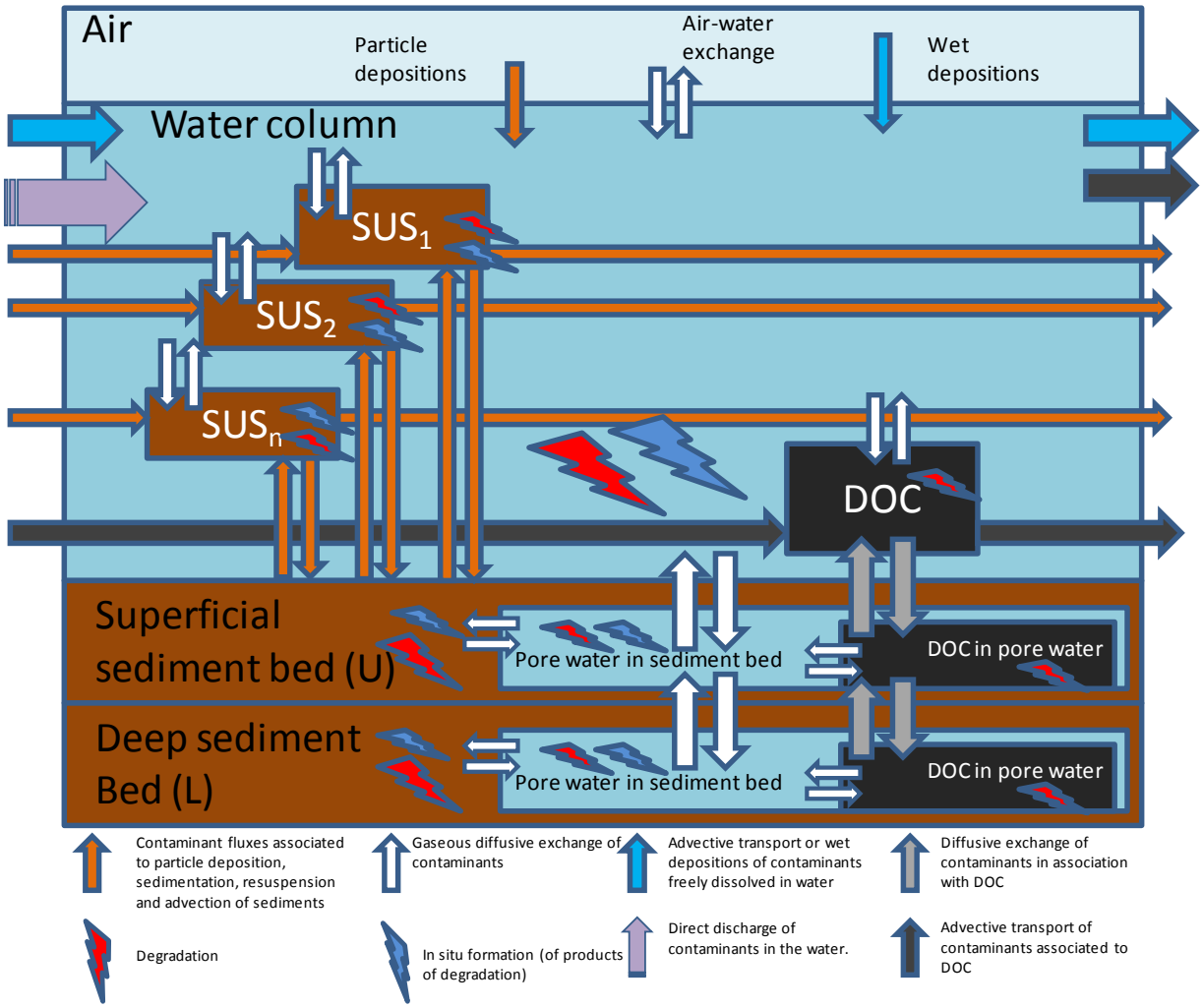

Figure SI2. Structure of the in-stream compartment, adapted from Nizzetto *et al.* (2016)[1, 2]

The structure of the INCA-contaminants in-stream model was illustrated in Figure SI2. The INCA-contaminants model takes into account information on river network structure, catchment topography, soil properties and land use. In the model, the in-stream phase is simulated as a group of several stream segments (reaches). In each reach the water column and the bed sediment are simulated as two different but interconnected compartments. The bed sediments are divided into superficial and deep layers. The depth of the superficial sediment bed is dependent on the in-stream suspended sediment transport dynamics (sediment deposition and mobilisation rates). Multiple sediment grain size classes can be simulated. For each grain size class, a mass balance is maintained based on the following processes: inputs from upstream reaches, entrainment with soil, flow erosion, sediment erosion, downstream advection and deposition of suspended sediment.[1] Mass balance calculations are based on those in the INCA-sediment model.[3]

The suite of possible inputs of contaminants to the in-stream system includes: wet and dry atmospheric deposition, diffusive air-water exchange, advection from upstream, possible point sources, and inputs from surface and diffuse runoff from the soil detailed at an arbitrary sub-catchment scale. The diffusive air-water exchange is dynamically calculated based on the inputs of wind speed and stream turbulence. After entering the water, the contaminants can be

in a truly dissolved phase (TDP), associated with DOC, or associated with suspended matter in the streams.[4] The partitioning of contaminants to suspended material in the water column is calculated separately for each grain size class, therefore the mass budget of contaminant bounded to solids is calculated individually per each class of sediment. Losses of contaminants from the in-stream system include: degradation of contaminants, formation of degradation products, and downstream advection.

2. References

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2. L. Nizzetto, D. Butterfield, M. Futter, Y. Lin, I. Allan and T. Larssen, Assessment of contaminant fate in catchments using a novel integrated hydrobiogeochemical-multimedia fate model, *Science of the Total Environment*, 2016, **544**, 553-563.

3. M. Futter, D. Butterfield, B. Cosby, P. Dillon, A. Wade and P. Whitehead, Modeling the mechanisms that control in - stream dissolved organic carbon dynamics in upland and forested catchments, *Water Resources Research*, 2007, **43**.

4. L. Nizzetto, G. Bussi, M. N. Futter, D. Butterfield and P. G. Whitehead, A theoretical assessment of microplastic transport in river catchments and their retention by soils and river sediments, *Environmental Science: Processes & Impacts*, 2016, DOI: 10.1039/C6EM00206D.