



Università degli Studi dell'Insubria
Dipartimento di Scienza e Alta Tecnologia
Como

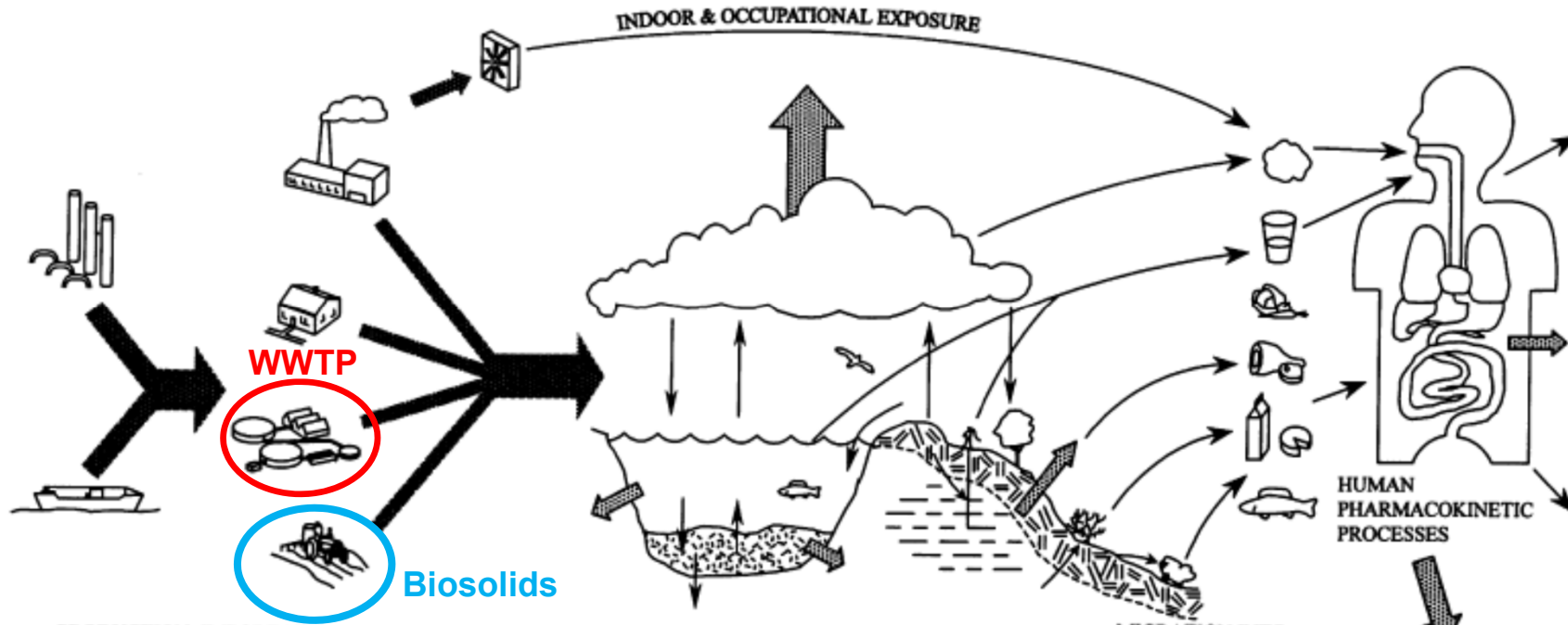
Perspectives on the environmental fate modelling of micropollutants

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Models in environmental fate study



1. Emission

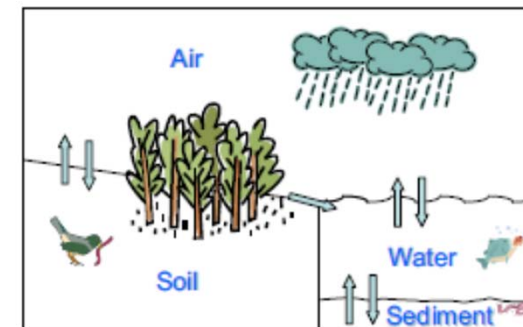
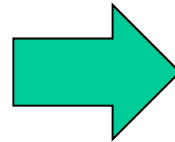
2. Environmental fate

3. Exposure

Modified from: Mackay, D., 2001. Multimedia Environmental Models: The fugacity approach. CRC press.

From scenario to model

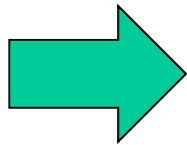
Design the scenario



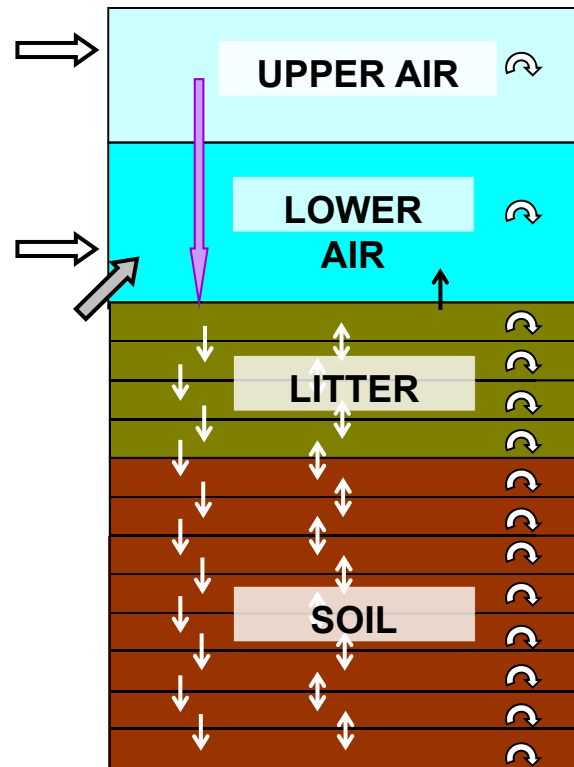
Di Guardo, A., 2014. Environmental Exposure Assessment, in: Encyclopedia of Toxicology. Elsevier, pp. 366–371.

From scenario to model

Build the Model

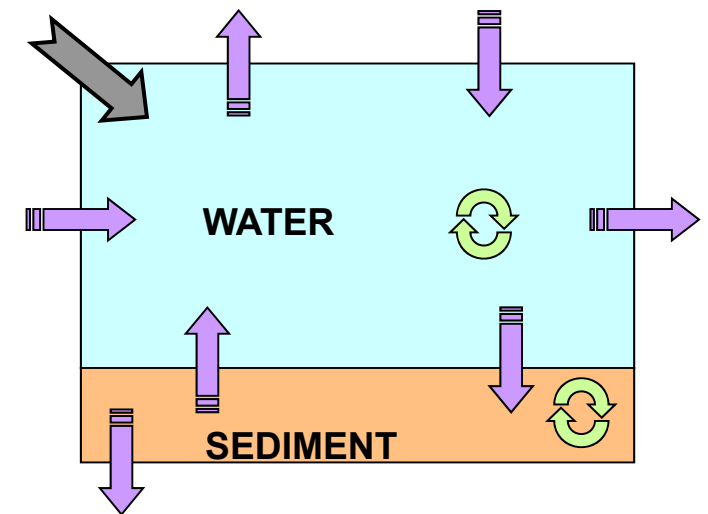


SoilPlus Model



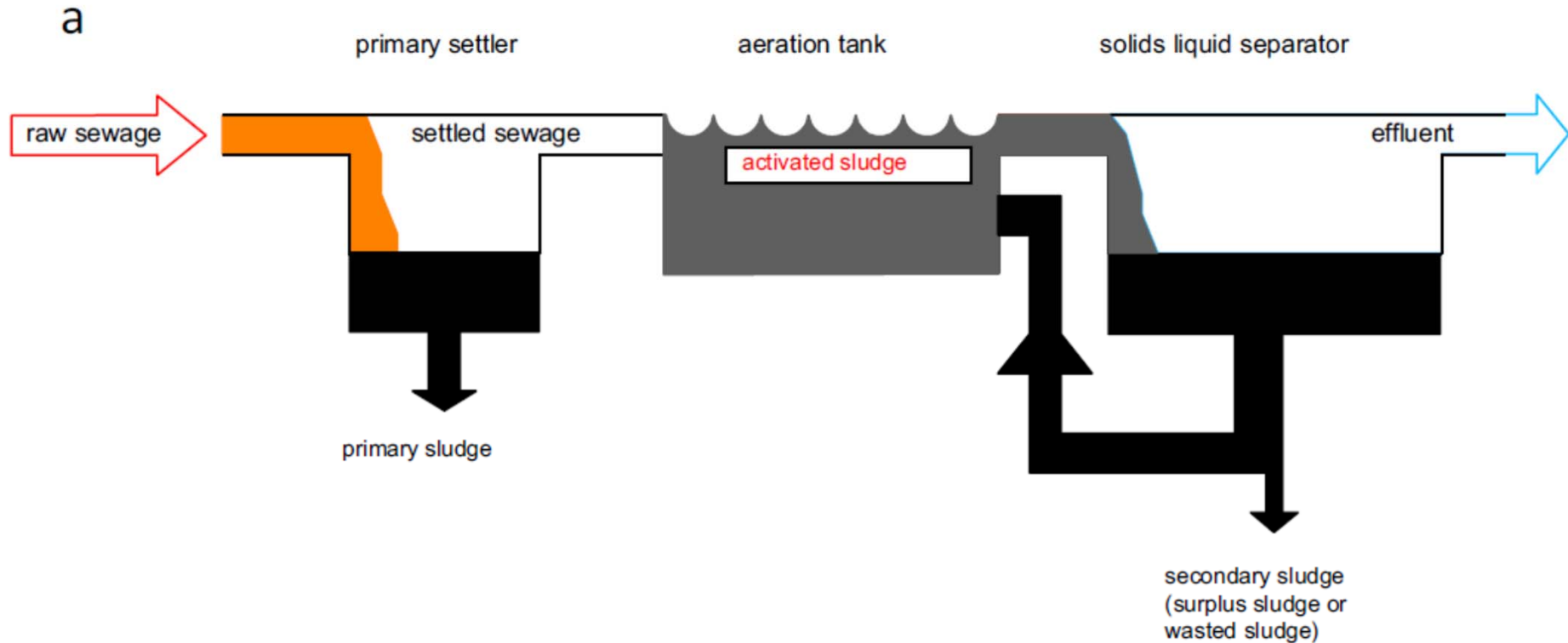
Ghirardello, D., Morselli, M., Semplice, M., Di Guardo, A., 2010. Environmental Science & Technology 44, 9010–9017.

Dyna Model



Di Guardo, A., Ferrari, C., Infantino, A., 2006.. Environmental Science and Pollution Research ,13, 50–58.

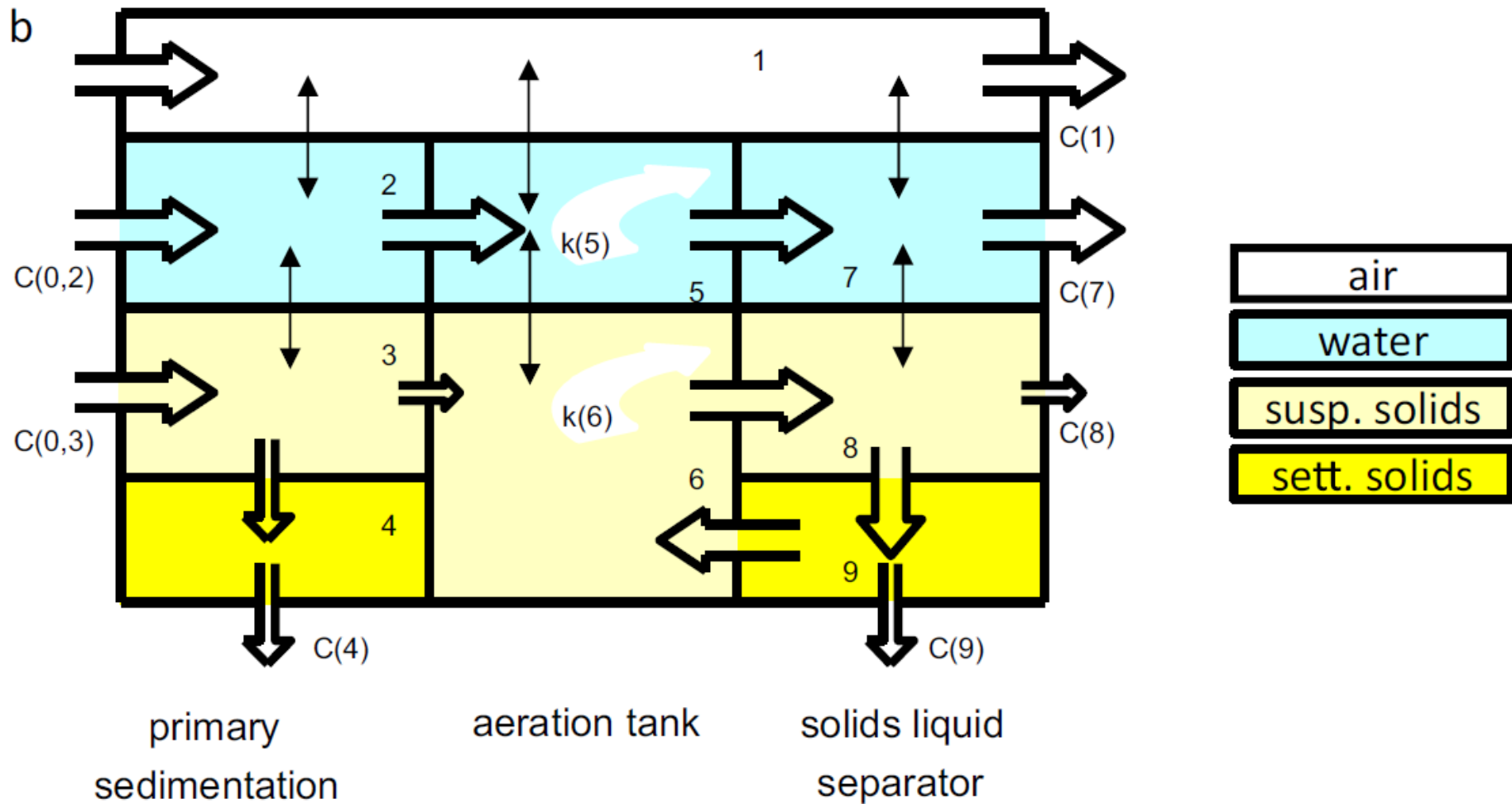
WWTP model: SimpleTreat



From: Struijs et al. (2016) Chemosphere 159, 619–627.



WWTP model: SimpleTreat



From: Struijs et al. (2016) Chemosphere 159, 619–627.

Problems and perspectives

- About 50% of the chemicals in REACH are **polar** and **ionized** (K_{ow} → K_d predictions are not valid)
- Only preliminary **estimation techniques for K_d of polar and ionized** chemicals are available → more research is needed
- Poor prediction of **degradation/adsorption** of micropollutants with the current techniques (Ozone/PAC/GAC) → e.g. influence of DOC
- **Degradation products** after micropollutant removal require additional investigations for modelling their fate (properties, half-lives, etc.)
- **Contaminant uptake in sludge and release to soil** require additional research for non polar chemicals

Thanks for your attention !

