Nanomaterial Fate and Exposure Modelling

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Nanotechnology industry is a fast-growing field, but still there is not a robust legislation about how nanomaterials can affect the environment. Anticipating this need, the Biorima (BIOmaterial RIsk MAnagement) project aims at developing a reliable methodology for better risk management of engineered nanobiomaterials. We present here the fate and exposure models developed within the mentioned project.

The nanobiomaterials are engineered nanoparticles (ENP) specifically designed to interact with biological systems with a medical purpose - either in Advanced Therapy Medicinal Products (ATMP) or Medical Devices (MD).

Different fate and behavior models have been developed over the years, being SimpleBox4nano [1] and MendNano [2] two of the most representative ones. These models evaluate the nanomaterials fate from two different points of view: SimpleBox4nano is based on mechanistic formulations of the key processes, while MendNano is based on empirical partitioning of the data.

The fate model needs to know the estimated emissions as an input, coming from a Material Flow Analysis (MFA) in Biorima. As the project is based on the release of nanobiomaterials, they are liberated mainly to water via excretion, hospital waste or residuals, and accidental release. It is also needed to consider the properties of the nanobiomaterials (such as density or diameter), as well as the environmental variables (like mean temperature, volumes, diffusivities…).

From here, a full study of the fate and behavior of the nanoparticles has been done. The main approach is to calculate specific constants, such as removal and transport rates for each component, and use them to calculate the concentration of a nanobiomaterial over time. With the obtained data, it is also possible to calculate the Predicted Environmental Concentration (PEC). Figure 1 is a representation of the model.

Different processes have been taken into account: Sedimentation, resuspension, burial, dissolution and aggregation.

- Sedimentation as a transport process between water and sediment compartments, modelled through a derivation of the Stokes' Law from gravitational settling of particles.
- Resuspension, which is the contrary process of sedimentation, involving the transport of the nanobiomaterial from sediment again to water.
- Burial is a removal process where the nanobiomaterial goes out of the system.
- Dissolution has been considered as a removal process in water and sediment compartiments. It depends on the surface of the particle and the chemical properties of the surrounding material. Noyes-Whitney equation has been applied.
- Both aggregation and attachment to larger particles have been also considered. It highly depends on collision frequencies which are described as a function of the particle size, density, number of concentrations of the particles present and characteristics of the surrounding material.

Biorima fate and behavior model implements all this information and starting from a particle emission, it can calculate the predicted environmental concentration and give it as an output of the model.

References

[1] Meesters, J. A., Koelmans, A. A., Quik, J. T., Hendriks, A. J., & van de Meent, D, Environmental science & technology, 48(10) (2014) 5726-5736.

[2] Liu, H. H., & Cohen, Y, Environmental science & technology, 48(6) (2014) 3281-3292.

Figures

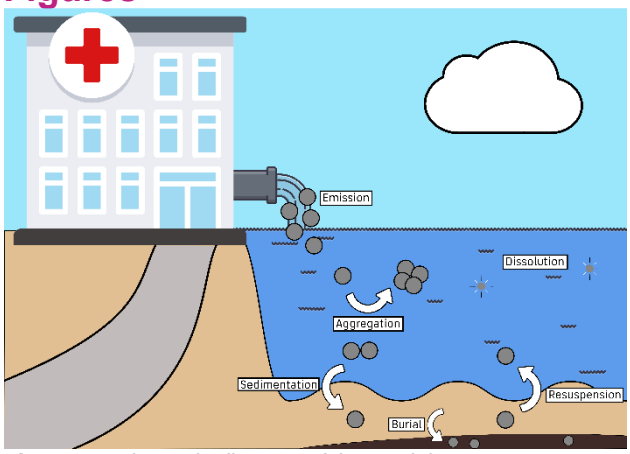

Figure 1. Schematic diagram of the model