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Physiologically Based Kinetic Modelling applications in Chemical Risk Assessment

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Physiologically based kinetic (PBK) modelling, which mathematically represents the body of a given species using chemical-specific and physiological information, is a fast-growing tool in toxicology. With this presentation, a perspective on the evolution of this tool, together with learning principles, will be given. The first part will introduce elements and a step-by-step process to develop a PBK model using the Open System Pharmacology Suite (OSPS)- PK-Sim platform. Briefly, an introduction to the building blocks and the equations representing the tissues in the body will be presented along with relevant exposure routes. The second part of the talk will be on the application of the tool and the extrapolations that can inform chemical risk assessment, especially with insight into the quantitative in vitro to in vivo extrapolations (QIVIVE). This approach is defined as the extrapolation of in vitro effect concentrations to in vivo bioequivalent exposures; the approach is considered a new approach methodology (NAM) and can be applied in different industrial sectors. The presentation will end with the recent recommendations from the ECETOC IVIVE workshop (Najjar et al. 2022; <https://doi.org/10.1007/s00204-022-03356-5>), to improve regulatory adoption to gain confidence in PBK modelling for QIVIVE in regulatory use.

Keywords:

PBPK model, QIVIVE, Human and Environmental Health.