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**XIII Encontro Nacional de
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IV Reunião do Grupo do Carbono

BOOK OF ABSTRACTS

15-17 June 2026
ISEL, Lisboa, Portugal



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**Sociedade Portuguesa
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O48 Modelling micropollutant adsorption in water treatment

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Micropollutants are increasingly recognized as a relevant challenge in both drinking water treatment and wastewater treatment, due to their widespread occurrence, persistence, and potential impacts on human health and aquatic ecosystems. Among the available treatment options, adsorption onto activated carbon remains one of the most robust and widely applied approaches for the removal of a broad range of organic micropollutants¹.

Adsorption-based micropollutant removal is currently applied in different process configurations in both drinking water treatment and wastewater treatment¹. In drinking water treatment, activated carbon (AC) may be used as powdered activated carbon (PAC) combined with coagulation/ flocculation/sedimentation, in hybrid systems integrating PAC and membrane processes or in granular activated carbon (GAC) filtration. In wastewater treatment, adsorption is commonly implemented as PAC dosed into activated sludge systems or as PAC or GAC post-treatment step after biological treatment. These different configurations create distinct operational conditions and demanding modelling needs.

To support process understanding, prediction and design, emphasis is placed here on mechanistic modelling of adsorption, namely through the Homogeneous Surface Diffusion Model (HSDM), which provides a mechanistic-based description of mass transfer and intraparticle diffusion². A critical aspect in real water matrices is competition between target micropollutants and background organic matter for adsorption sites, which dramatically reduces adsorption capacity and modifies removal behaviour relative to ultrapure water conditions. This effect can be addressed through the Equivalent Background Compound³ or the Tracer models⁴, based on the Ideal Adsorbed Solution Theory, enabling competition to be incorporated into mechanistic adsorption modelling while retaining engineering applicability. A suitable experimental-modelling workflow starts with batch isotherm and kinetic tests, followed by parameter estimation, model calibration, prediction under relevant operating conditions, and validation against independent data. By coupling these calibrated adsorption models with mass balance equations, the removal efficiency of micropollutants can be predicted at environmentally relevant concentrations (ng/L)³.

Overall, modelling of micropollutant adsorption can support several practical objectives, including AC selection, the development and screening of new adsorbents, and the design and optimisation of treatment processes. The proposed modelling approach will be illustrated with datasets from several research projects, highlighting its applicability across different treatment contexts.

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