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Individual-based modelling elucidates about the role of nanomaterials on methane production

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Modelling stands as a potent tool for the simulation of real-world systems, offering predictive insights into their dynamic behaviours. Individual-Based Models (IBMs), with their ability to capture intricate details at the microscale, emerge as particularly valuable tools. In the context of anaerobic digestion (AD), the application of IBMs gains significance. Some nanomaterials (NM) enhance methane production in anaerobic ecosystems, by yet unknown mechanisms. This study employed IBMs through the NUFEB software to investigate possible mechanisms of action by NM in AD. The models incorporated Monod-based growth dynamics for methanogenic-based growth and production of extracellular polymeric substances, a Lennard-Jones interaction between NM and microorganisms for simulating attachment, and Hooke forces between microorganisms and themselves and EPSs to simulate the attachment between biological entities and formation of biofilms. The simulations also explored boundary conditions (Dirichlet or Neumann), considering scenarios of both open systems and closed environments. Shear force was introduced as a variable to assess its impact on microbial behaviour, and different shapes of NM were simulated, differentiating between smaller and larger particles, and smoother and rougher surfaces. Results indicate that the rugosity of the material plays a pivotal role in providing increased surface area for microorganism attachment. In open systems, higher rugosity leads to the displacement of microorganisms, exposing them to the environment while concurrently attached to NM. These displaced microorganisms have higher access to their substrate and produce more methane. Conversely, in closed systems, a more rugous material serves as a protective shield, reducing the washout of organisms under the influence of shear force. With more microorganisms remaining in the system, more methane is produced. This research provided valuable insights into the role of NM morphology in shaping microbial interactions during AD. The findings enhance our understanding of the complex interplay between NM structures and microbial populations, providing essential knowledge for the optimization of AD processes in the presence of NM.