# 2023_06_Generating an energy-mass-information equivalence simulator for waste-to-energy non-classical bioprocessing optimisation

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## (a) Motivation for the project

Waste-to-energy technologies are infinitely interesting as a sustainable approach to deal with waste management while also providing renewable energy. Among these technologies, anaerobic digestion (AD) is a promising option for the treatment of organic waste. One of its limiting steps is the is the conversion of short chain fatty acids (VFAs) to methane by a syntrophic association between syntrophs and methanogens. This involves with syntophs intelligence to decide effective VFAsâ€™ transformation. Such microbial intelligence will be formulated using the mass-energy-information principle for unprecedented optimal operating conditions. The feature of this project is to include syntophs intelligence (i.e., information for microbial decision making for their own survival or/and syntrophic relationship with methanogens). By enabling the optimisation of anaerobic digesters, this simulator could contribute to reducing the environmental impact of organic waste while providing a renewable energy source. As a second-year biochemist with a passion for data science, delving into this interdisciplinary topic offers a unique opportunity to expand my knowledge and skills. It brings together individuals from diverse academic backgrounds to solve questions with a huge impact on understanding cell-to-cell interactions and revolutionizing waste management and sustainability.

## (b) Context and background

The on-going research towards sustainable fuel production entails the improvement of the microbial catalysts involved. The possible reversibility of specific anaerobic catabolic reactions opens a range of possibilities for the development of novel reductive bioprocesses. These reductive biohydrogenation pathways enable the production of high energy density chemicals of interest as biofuels such as methane, alcohols and long chain fatty acids. Overall, analysing the potential reversibility of catabolic pathways therewith contributes to the development of efficient and reliable anaerobic bioprocesses to produce biofuels and chemicals.

The topic I have chosen is related to topics from the REP scheme and NERC remits such as Environmental microbiology, All aspects of environmental influence on, and effects of, microbial systems; bioremediation; microbial diversity, pollution, waste, and resources.

## (c) Objectives and methodology

The objective is to build a Maxwell's demon intelligence (simulation) model in anaerobic bacteria including the balance of mass, energy, and information (bacterial intelligence decision making). Though this will be able to investigate the potential reversibility of specific anaerobic pathways of interest. The energy-mass-information equivalence of the different steps in biochemical pathways are analysed and combined with assumptions concerning kinetic and physiological limitations to figure out whether pathways are potentially reversible by imposing changes in process conditions. Anaerobic bioprocesses take place under energy scarcity conditions due to the absence of electron acceptors, and result to metabolic pathways involving reduced chemicals. Metabolic reactions occur close to thermodynamic equilibrium with minimum energy waste and consequently, environmental changes in product and substrate concentrations can easily reverse the driving force of the chemical reaction catalyzed.

The energy-mass-information equivalence simulation that will allow us to investigate the above will be built based on Mitchellâs chemiosmotic theory including the Î of ATP synthesis and Î”G of the Maxwell demon.

The project will involve the validation of the model using an experimental dataset from the PIâs lab, specifically a syntrophy for waste-to-energy anaerobic digestion that has been collect

**Project length:** 6 weeks