

An individual-based model for the study of *Paracoccus denitrificans*, a denitrifying bacterium

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Agriculture is viewed as a contributor to greenhouse gas emissions, one of the causes of global warming. The use of nitrogen based fertilisers has also been identified as one of the major factors in this process. CO₂ emissions are relevant, but in the case of agriculture, the most important are N₂O emissions. Consequently, understanding the environmental factors that control N₂O production and consumption by microbes is critical and a challenge to the development of practical mitigation strategies for N₂O emissions [1].

The individual-based model INDISIM, a computational model to study bacterial cultures, together with its different versions have been used successfully to deal with diverse biological systems where microorganisms are the main agents driving the behaviour of these systems [2-4].

The main goals proposed in this work are: i) Design and description of a bacterial model for *Paracoccus denitrificans*, one of the most important denitrifying bacteria in soils, and a culture medium in which it develops and grows (batch or continuous culture) in the context of the individual-based model methodology, identifying the main factors involved in the denitrification process driven by this microbe. ii) Implement the model in NetLogo, a free access multi-agent programmable modelling environment, and compare the simulation outputs with some experimental work.

A virtual bioreactor for *P. denitrificans* was designed using a culture medium containing succinate as a carbon source, ammonium as nitrogen source and various electron acceptors such as oxygen, nitrate, nitrite, nitrogen monoxide and dinitrogen oxide. INDISIM was the core model for the bacterial behaviour and five metabolic pathways were selected and translated into balanced chemical equations using the Thermodynamic Electron Equivalents Model Two (TEEM2) [5]. This thermodynamic approach is the basis of the individual activities that this microbe carries out for its cellular maintenance and production of new biomass by using the substrates in the medium.

The preliminary simulation results achieved with this NetLogo simulator showed that it is possible to work with this virtual bioreactor, which is prepared to formulate various initial culture media, adjust the dilution ratio, fix the initial number of viable microorganisms, specify duration of the evolution, set the level of oxygen dissolved in the medium to the use of aerobic or anaerobic metabolic pathways, among other options. Some of the outputs regarding the temporal evolutions of the diverse substrates in the medium are consistent with previous experimental data carried out with *P. denitrificans* [1], which indicates that this type of computational model jointly with TEEM2 offer a new strategy for the study and understanding of denitrifying bacterial activity.

Keywords: Denitrification, *Paracoccus denitrificans*, Individual-based model, Thermodynamic Electron Equivalents Model, NetLogo

References

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