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INDISIM-Paracoccus, an individual-based and thermodynamic model for a denitrifying bacterium

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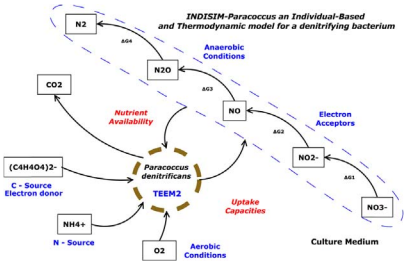
HIGHLIGHTS

- An IBM to study denitrification that uses thermodynamics for the cellular activity.
- The simulator facilitates interaction between modelers and experts in denitrification.
- The thermodynamic properties embedded into individual cells for modeling.

GRAPHICAL ABSTRACT

The individual-based model approach with the thermodynamics embedded as an intracellular model defines the behavior-rule of the individual cell for maintenance and biomass generation to study the denitrification products dynamics, especially the greenhouse gas N_2O, carried out by denitrifying bacterium Paracoccus denitrificans.



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ABSTRACT

We have developed an individual-based model for denitrifying bacteria. The model, called INDISIM-Paracoccus, embeds a thermodynamic model for bacterial yield prediction inside the individual-based model INDISIM, and is designed to simulate the bacterial cell population behavior and the product dynamics within the culture. The INDISIM-Paracoccus model assumes a culture medium containing succinate as a carbon source, ammonium as a nitrogen source and various electron acceptors such as oxygen, nitrate, nitrite, nitric oxide and nitrous oxide to simulate in continuous or batch culture the different nutrient-dependent cell growth kinetics of the bacterium *Paracoccus denitrificans*. The individuals in the model represent microbes and the individual-based model INDISIM gives the behavior-rules that they use for their nutrient uptake and reproduction cycle. Three previously described metabolic pathways for *P. denitrificans* were selected and translated into balanced chemical equations using a thermodynamic model. These stoichiometric reactions are an intracellular model for the individual behavior-rules for metabolic maintenance and biomass synthesis and result in the release of different nitrogen oxides to the medium. The model was implemented using the NetLogo platform and it provides an interactive tool to investigate the different steps of denitrification carried out by a denitrifying bacterium. The simulator can be obtained from the authors on request.

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1. Introduction

Denitrification is one of the key processes of the global nitrogen cycle driven by bacteria (Blackburn, 1990; Zumft, 1997). One of the reasons for studying denitrification is that it contributes to nitrous oxide (N_2O) emissions when denitrifying bacteria do not complete the metabolic pathway implicated (Davidson et al., 1991; Snyder et al., 2009). The global warming potential of N_2O is 296 times greater than a unit of CO_2 (Richardson et al., 2009). In agricultural soils, N_2O emissions are of great importance due to the large amount of N-fertilizer in crops and soil organic matter mineralization which depends on the conditions the microorganism encounters in its surrounding environment (Snyder et al., 2009; Woolfenden et al., 2013).

In conditions of low oxygen (O_2) availability, such as waterlogged soils, certain bacteria are able to use nitrate (NO_3^-) as a final electron acceptor and carry out respiratory metabolism in anaerobic conditions (denitrification). These bacteria are known as heterotrophic denitrifying bacteria and are widespread in agricultural soils (Felgate et al., 2012; Richardson et al., 2009). The bacterium *Paracoccus denitrificans* is one of the best-characterized prokaryotes and one of the paradigm species for studies of the biochemistry and regulatory biology of denitrification (Bergaust et al., 2010; Caspi et al., 2012).

To model the dynamics of a bacterial denitrification system with *P. denitrificans* at least three metabolic pathways must be considered as follows. In the aerobic phase it can execute "*Aerobic respiration*" with the oxygen (O_2) as the electron acceptor, and "*Nitrate reduction - Dissimilatory*" with nitrate (NO_3^-) as the electron acceptor (Baker et al., 1998; Beijerinck, 1910; Caspi et al., 2012), and in anoxic conditions it executes the "*Nitrate reduction - Denitrification process*" because it is capable of anaerobic growth in the presence of NO_3^-, nitrite (NO_2^-), nitric oxide (NO) or N_2O as electron acceptors (Baumann et al., 1996; Bergaust et al., 2010, 2012; van Verseveld et al., 1983).

The choice of a modeling approach to study a bacterial system, either population-level (top-down, usually continuous with differential equations) or individual-based (bottom-up, discrete and computational model) is an important decision depending on the project's specific aspects, the characteristics of the system and the questions to be answered (Ferrer et al., 2008). A number of denitrification models have been reviewed by Heinen (2006). Most of them incorporate a large number of parameters including NO_3^-, soil moisture, soil temperature and pH. The simplest models are obtained by adjusting empirical functions to the experimental results used for their studies. More recently, Kampschreur et al. (2012) and Woolfenden et al. (2013) published specific denitrification models describing the process carried out by microbes in terms of a set of differential equations according to Monod and Michaelis–Menten kinetics. Therefore, the population-level models deal with population variables and fix a set of governing laws (equations) which are based on, or at least consistent with, an assemblage of assumptions about the individual behavior of microbes.

Alternatively, it is possible to simulate the interactions of autonomous agents (individual and collective entities) and their environment, using agent-based models or, more specifically, Individual-Based Models (IBMs) that are defined by agents which model living entities (Grimm, 1999). IBMs have the ability to simulate variability among individuals, local interactions, complete life cycles and individual behavior according to the changing individual internal and external conditions, linking mechanisms at the individual level to behavior at the population level (Grimm, 1999; Mantzaris, 2007). IBMs consider individuals as discrete entities that follow behavior-rules that drive how the individuals interact with their surrounding environment and other individuals, so that the individual and the environment can change and adapt their characteristics over time. This makes it possible to explore connections between micro-level behaviors of individuals to macro-level patterns that emerge from their interactions (Prats et al., 2008; Wilensky, 1999).

The two approaches, the continuous-macroscopic and the discrete-microscopic approaches, are not incompatible or exclusive, but are complementary. Population-level approaches are mostly used for predictive purposes, due to their simplicity and computational efficiency. Moreover, they have been widely tested and, nowadays, many modeling frameworks exist. IBMs have had their own place in microbial research and have also been used for some predictive purposes, but their strength lies in the means they offer to disentangle and understand the dynamics of bio-systems (Hellweger and Bucci, 2009; Kreft et al., 2013).

In summary, in addition to the characteristics just described, IBMs are useful to study the relations between experimental data and theoretical proposals, allowing testing of the consistency of different microbial models, and supplying holistic knowledge of the systems under study (Ferrer et al., 2008).

Ginovart et al. (2002) developed a discrete simulation model to study bacterial cultures called INDISIM. This model has been used as the core for other models such as INDISIM-SOM (Ginovart et al., 2005), INDISIM-YEAST (Ginovart and Cañadas, 2008), INDISIM-COMP (Prats et al., 2010) and INDISIM-Saccha (Portell et al., 2014) to deal with soil organic matter dynamics, to study yeast fermentations and multi-species composting, and to analyze the dynamics of *Saccharomyces cerevisiae* anaerobic cultures, respectively. For a review of some microbial system evolutions using the IBM methodology see, for instance, (Bley, 2011; Ferrer et al., 2008; Hellweger and Bucci, 2009; Kreft et al., 2013; Lee et al., 2009; Resat et al., 2012).

Several approaches have been reported to develop a rigorous thermodynamic description for biomass yield prediction (Christensen and McCarty, 1975; Heijnen and Van Dijken, 1992; Liu et al., 2007; Maskow and von Stockar, 2005; McCarty, 1971; Rittmann and McCarty, 2001; Tijhuis et al., 1993; von Stockar and van der Wielen, 1997; Xiao and VanBriesen, 2006). These approaches consider the Gibbs energy for cell synthesis from C-sources and N-sources, the energy available from substrate transformation, the specific Gibbs energy consumption for cellular maintenance, and the energy efficiency transfer to the overall process to describe growth of micro-organisms in a standard mathematical and thermodynamic model.

To tackle and understand the environmental factors that control the denitrification process it is convenient to investigate the bacterial denitrification dynamics in a controlled environment such as a bioreactor (Baker et al., 1998; Baumann et al., 1996; Felgate et al., 2012; Richardson et al., 2009). In this paper we will: (i) Design, implement, and parameterize thermodynamic behavior-rules for a *P. denitrificans* model in the INDISIM methodology context; (ii) Simulate a bioreactor containing a culture medium where *P. denitrificans* develop and grow in order to mimic the experimental protocols presented by Felgate et al. (2012); and (iii) Investigate the effects of the priority in the use of different electron acceptors at the microbial level formulating two hypotheses about the order in which the reactions are followed by the bacteria *P. denitrificans* while the denitrification process occurs, and test these hypotheses with the simulator developed, comparing the simulation outputs with experimental data reported in Felgate et al. (2012).

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