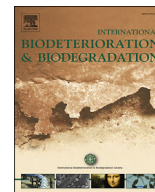




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Next generation modeling of microbial souring – Parameterization through genomic information

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ABSTRACT

Biogenesis of hydrogen sulfide (H₂S) (microbial souring) has detrimental impacts on oil production operations and can cause health and safety problems. Understanding the processes that control the rates and patterns of sulfate reduction is crucial in developing a predictive understanding of reservoir souring and associated mitigation processes. This work demonstrates an approach to utilize genomic information to constrain the biological parameters needed for modeling souring, providing a pathway for using microbial data derived from oil reservoir studies. Minimum generation times were calculated based on codon usage bias and optimal growth temperatures based on the frequency of amino acids. We show how these derived parameters can be used in a simplified multiphase reactive transport model by simulating the injection of cold (30 °C) seawater into a 70 °C reservoir, modeling the shift in sulfate reducing microorganisms (SRM) community composition, sulfate and sulfide concentrations through time and space. Finally, we explore the question of necessary model complexity by comparing results using different numbers of SRM. Simulations showed that the kinetics of a SRM community consisting of twenty-five SRM could be adequately represented by a reduced community consisting of nine SRM with parameter values derived from the mean and standard deviations of the original SRM.

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1. Introduction

Microorganisms play key roles in the life cycle of oil and gas formation, production, and bioremediation (Head et al., 2003, 2014; Youssef et al., 2007, 2009). During secondary oil production, seawater with typical sulfate concentration of ~28 mM, is often injected into oil reservoirs to maintain reservoir pressure and sweep out oil, potentially giving sulfate reducing microorganisms (SRM) the opportunity to couple the reduction of sulfate to bisulfide (HS⁻) with the biodegradation of crude oil derived organics, such as volatile fatty acids (VFAs), aromatics (e.g. toluene) and aliphatic hydrocarbons. The sulfide produced by this process (also known as microbial souring) presents significant corrosion (e.g. sulfide stress corrosion cracking of carbon steel infrastructure), health and safety, and economic problems to oil producers (Fuller

and Suruda, 2000; Vance and Thrasher, 2005; Semcrude, 2011). Understanding and preventing souring is therefore an ongoing priority for the industry.

Reservoir models are essential management tools used across the oil industry to understand and predict fluid flow in the subsurface during different stages of oil production. Increasingly, accurate representation of souring has become a priority (Haghshenas et al., 2012). This is not a trivial problem, as the process of water injection into an oil reservoir develops gradients in a range of important environmental characteristics, and these gradients vary in time and space as water injection continues. For example, the injection of relatively cold seawater into a hotter reservoir produces gradients in temperature, sulfate (due to high concentrations in the injected seawater), and electron donor (higher crude oil derived organics in the formation water than the injection water). All of these dynamic, intersecting gradients provide a wide range of potential ecological niches for different SRM, potentially leading to a diverse community which develops and changes through time and space as the changing environmental

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conditions imposed by water flooding preferentially select for certain SRM over others as demarcated by their physiological characteristics (or traits). Most modeling studies assumed that the kinetics of the diverse SRM can be effectively represented by a single set of kinetic parameters (e.g. maximum growth rate and half saturation constant for electron acceptors and donors). Models of experiments conducted under constant environmental conditions further assume the kinetic parameter values to be constant (e.g. constant maximum growth rate under isothermal conditions) (Cheng et al., 2016). Under this scheme, 'optimal' values of the kinetic parameters are systematically derived from calibrations that fit observed data. While computationally simple, such representations are far from reality. Microbial communities are typically diverse and their distributions stochastic. Within natural communities, organisms thrive by maximizing their fitness relative to their environmental conditions and other competitors. Community composition is therefore an emergent property that constantly evolves as communities self-organize in response to heterogeneous environmental conditions. When each organism maximizes its own growth, they collectively maximize the rate of a given process (e.g. sulfate reduction) under the prevailing environmental condition. It is therefore important for models to sufficiently capture the microbial complexity that can potentially emerge under these fluctuating conditions. Insufficient complexity runs the risk of diminishing the predictive power of a model as conditions and gradients evolve through time, whereas too much complexity increases computational demands and may be under-constrained by available data. To investigate this problem of complexity we take advantage of two rapidly developing fields: increased sophistication in modeling microbial processes, and the greater utilization of microbial genomics providing understanding of microbial function and diversity in the environment.

Microbial models that predict the structure and activity of the microbial community on the basis of physiological and ecological traits of different microbial guilds have increasingly gained traction as approaches for further understanding the response of a microbial community to perturbation (Le Roux et al., 2016) or to better represent microbial function in more established models (Follows et al., 2007). The increasing utilization of a trait-based approach lies in the advantages of reducing the complexity of the microbial community to several different functional guilds on the basis of traits related to substrate utilization, growth, carbon use efficiency and their response to environmental factors (e.g. temperature). Parameterizing different combinations of these traits can determine an individual organism's fundamental niche (Holt, 2009). The realized niche is then determined through competition with different modeled microbial guilds for common substrates (electron donors or acceptors). This reductionist approach can therefore discreetly reproduce the functional basis of a given microbial community without the computational intractability or ecological redundancy of representing all of the individual microorganisms.

Souring, as a microbially mediated process, is inherently amenable to representation through trait-based modeling. Both traditional isolation experiments and more recent genomic data provide abundant data on the physiological mechanisms that may be used to develop and parameterize trait-based models, including, for example, the range of electron donors the SRM may use (Muyzer and Stams, 2008). An important flexibility that may be represented by trait-based modeling frameworks is the competition by different functional guilds (e.g., denitrifiers and SRM) and linked processes (e.g., SRM and sulfide-oxidizing bacteria) that can lead to estimates of net production of sulfide, rather than bulk production rates. More recent proliferation of genomic data sets provides a wealth of potential data that can be used to identify specific traits of organisms. Significant advances in the identification and annotation of complex

(meta)genomic data sets (e.g., Wu et al., 2014) make the derivation and parameterization of key traits possible.

This work seeks to provide a way forward to more accurately represent oil reservoir microbial dynamics, thereby improving predictions of biogenic souring. To do this we first show how genomic information can be used to constrain the biological parameters needed for modeling souring, providing a pathway for using microbial data derived from oil reservoir studies. We then show how these derived parameters can be used in a simplified reactive transport simulation of seawater injection into a reservoir. Finally, we explore the question of necessary model complexity by comparing model results using different numbers of sulfate reducers.

2. Methods

2.1. Deriving model parameters from microbial datasets

Genomic data provides insights related to important traits that can be used to constrain the parameterization of the current generation of models. While there are multiple traits that can be derived from genomic data, optimal growth temperatures and minimum generation time have been shown to have good correlation to observational data. The generation time of individual groups within a guild is an important trait in the models, and can be estimated by examining the codon usage bias evident within highly expressed genes from individual genomes (Vieira-Silva and Rocha, 2010). Similarly, another important trait, the optimal growth temperature, is found in the preferential use of several amino acids, for which the corresponding signatures may also be discerned from the genomes (Zeldovich et al., 2007).

Minimum generation (doubling) times were predicted based on codon usage bias between all genes and in a set of highly expressed genes following the linear regression model from (Vieira-Silva and Rocha, 2010). We used ribosomal protein genes as the set of highly expressed genes. Genome sequences for twenty-five SRMs were downloaded from Genbank genomes (<ftp://ftp.ncbi.nih.gov/genomes/Bacteria/>) (Table 1). (Note: Only closed genomes were downloaded). Genes and their annotations were extracted from annotation files (.ppt files) and genes for ribosomal proteins were identified based on the annotation fields. Using the nucleotide sequences for the two set of genes, codon usage bias index, $\Delta ENC'$, was calculated using the following equation:

$$\Delta ENC' = \frac{ENC'_{all} - ENC'_{ribosomal\ protein\ genes}}{ENC'_{all}} \quad (1)$$

where ENC' is the effective number of codons given G + C composition (Novembre, 2002) and inputted to the above equation. Optimal growth temperature was calculated based on the frequency of amino acids IVYWREL in the proteome of the organism as in (Zeldovich et al., 2007). We conducted literature searches to acquire data on optimal growth temperature and minimum generation times for SRM. Data on eleven SRM were acquired for comparison against derived minimum generation times and optimal temperatures from genomic data. The SRM belong to the genus: *Archaeoglobus*, *Desulfatibacillum*, *Desulfococcus*, *Desulfosporosinus*, *Desulfovibrio*, *Desulfurococcus*, *Sulfurimonas*, *Thermodesulfobacterium* and *Thermodesulfobium* (see Table 2).

Kinetics of microbial growth under substrate limitation can be described by Monod equation (see Equation (3)). An important parameter in the Monod equation is the half saturation constant, K_s , which represents the affinity of the microbe for a particular substrate. Kinetic studies of dissimilatory sulfate reductions revealed a broad range of values of half saturation constants (sulfate),

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