

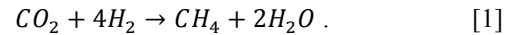
**THE ROLE OF CELL MEMBRANES IN COUPLED GEOCHEMICAL-BIOENERGETIC MODELING.**

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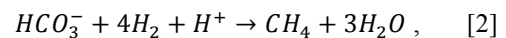
**Introduction:** Energy availability is anticipated to be a key determinant of habitability in environments that lack direct access to sunlight or the products of photosynthesis. Typically, such availability is quantified in terms of the Gibbs energy change represented in potential metabolic reactions, but this is an incomplete description of how energy constrains biological potential. Our work is designed to quantify energy *flux* which, in turn, constrains the rate of biosynthesis and the abundance of biomass that can be supported in steady state. In our work, a geochemical model (EQ3/6) is coupled to a cell-scale reactive transport model. Such a model can predict concentration distributions (and thus  $\Delta G$ ), substrate fluxes, and reaction rates at the sub-micron scale, based on well-established physical principles of transport laws and conservation of mass [1].

The cell membrane is critical in mediating substrate flux and the accuracy of the cell-scale reactive transport model depends on correctly representing its properties within the model construct. The biological cell contains three basic structural units: cell wall, cell membrane, and cytoplasm. The cell wall imparts shape and rigidity to the cell, but is freely permeable to low molecular weight ions and molecules. Its purpose is to define the boundary between the external and intracellular environment. The cell membrane is sandwiched between the cell wall and cytoplasm and serves as the cell's osmotic barrier. Small uncharged molecules such as H<sub>2</sub> and CO<sub>2</sub> readily diffuse through the cell membrane, whereas ions such as HCO<sub>3</sub><sup>-</sup>, CO<sub>3</sub><sup>2-</sup>, and SO<sub>4</sub><sup>2-</sup> cannot. However, a variety of mechanisms exist by which charged substrates are conducted across the membrane; here, we describe an approach to accurately represent cross-membrane substrate during methanogenic CO<sub>2</sub> reduction.

**Membrane modeling:** The model simulates ion translocation by allowing specific ions to diffuse through the membrane at a rate that is commensurate with the fraction of the cell surface that contains appropriate channels (see below). We assume that metabolic reactions for methanogenesis occur in the cytoplasm and at the inner membrane surface, but not in the cell wall. The reaction representing methanogenic CO<sub>2</sub> reduction can be written in terms of uncharged species that will diffuse freely across the membrane:



In such a case, substrate transport can be quantified simply, via a (slightly) modified diffusivity within the membrane, but with the entire membrane surface area accessible to substrate transport. However, cross-membrane transport is not as simple for a cell undertaking



because the ionic species ( $S_i$ ) such HCO<sub>3</sub><sup>-</sup> and H<sup>+</sup> cross the membrane only through trans-membrane proteins (porins). Porin open channels constitute 0.75% of the cell surface [2] so to mimic this, the membrane diffusion coefficient of  $S_i$  is taken as 0.75% of the diffusion coefficient of  $S_i$  outside of the cell. Additionally, the homeostasis of pH within the cell must be maintained. In proton-consuming reactions (e.g., [2]), the cell must additionally pump in protons from the exterior against a pH gradient, representing an energetic cost that must be factored into the calculation of metabolic energy balance.

**Modeling results:** We present a quantitative comparison of the metabolic energy balance for methanogens using the membrane transport strategies represented in Eqs. 1 & 2. Applying this comparison across a range of pH, H<sub>2</sub>, and  $\sum CO_2$  that reflects the potential variability within serpentinizing systems demonstrates that the strategy of Eq. 1 is viable and in some cases preferential at moderate pH and high  $\sum CO_2$ , but that ion-translocating mechanisms become essential for the viability of methanogenesis at the high pH and low  $\sum CO_2$  values that often characterize serpentinizing systems.

**References:** [1] Alperin, M and Hoehler, T. (2009) *Am. J. Sci.* 309, 869-957. [2] Madigan et al. (2003) *Brook biology of microorganisms.*

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