Supplemental Information

**OBJECTIVE**

We conducted a numerical modeling study to explore how different soil textures, environmental conditions (soil water content, temperature), and methane (CH4) leak rates affect the transport and distribution behaviour of CH4 gas in surface soils. We designed this study to explore how variation of these parameters can influence two common measurement techniques used to address fugitive gas migration: (1) in-soil CH4 concentration and (2) surface CH4 flux rates. We sought to make observations from the model environment that could explain phenomena seen in the field, and better equip future field measurement campaigns.

**VERTICAL (1D) DIFFUSIVE SOIL GAS TRANSPORT MODEL**

We built a model domain which simulated the upper 1 m of surface soil and the overlying atmospheric layer. The soil profile was subdivided into ten layers of uniform depth. We simulated CH4 entering the base of the soil profile, biological production of CH4 and the vertical diffusion of both sources through the soil and to the atmosphere.

**GOVERNING EQUATIONS**

Gas transport in upper soils around the soil-atmosphere boundary region is dominated by (1D) vertical diffusion, as gaseous species move along concentration gradients from high to low (Huggett, 1975; Kühne et al., 2012). We modeled diffusive transport of CH4 through the upper 1 m of soil was modeled using Fick’s Second Law. We also added a production function to simulate biological CH4 production within the soil (Nickerson and Risk, 2009; Pumpanen et al., 2003). The equation is detailed below:

(1)

where *C* is the “in-soil” concentration (ppm) of CH4 within each soil layer, *t* is time (s), *z* is depth (m), is soil gas diffusivity (m-2 s-1) and is biological CH4 production (µmol CH4 m-2 s-1) relative to depth. To solve for flux (µmol CH4 m-2 s-1) between adjacent soil layers, and at the soil-atmosphere boundary, equation (1) was discretized with Euler’s method under a time step series of 1 s (Nickerson and Risk 2009):

We calculated the concentration of CH4 within each soil layer at every time step by following Pumpanen et al. (2003) and Nickerson and Risk (2009):

(2)

where is the CH4 concentration in each layer at the last time step, at time zero, initial layer CH4 concentration is equal to the concentration of CH4 in the atmospheric layer (), which is held constant at 2 ppm, thus (), is air-filled porosity of the soil, is total soil depth divided by the number of layers, is flux out of the layer below, and is the flux leaving the layer in question. Recall that is the biological production of CH4 within the layer.

Biological CH4 production was not evenly distributed throughout the profile. We modeled to decrease as a function of depth because the majority of biological CH4 production occurs in the uppermost layers (~ 10 cm) of the soil profile where organic material such as plant litter accumulates (Pietikäinen et al. 1999). follows an exponential decrease by a factor of *e*,referred to as *e*-folding or damping depth *η*, or the depth at which falls to 1/*e* of its value at the surface (Bowling et al., 2015; Davison et al. 2006; Lloyd et al. 1994, Nickerson and Risk 2009).

Thus, the total biological CH4 productionwithin the soil profile is equal to the sum of in each layer adjusted for depth and *e-*folding:

(3)

where is the biological production in each layer (recall is the number of layers) at depth , and is the depth over which production falls by 1/*e*.

We simulated three unique soil textures to approximate different types of soil which could occur in the field. Soil texture is important because, within the soil matrix, solid and liquid obstacles can reduce the cross-sectional area and increase the mean free path length for diffusing gas molecules (Sallam et al. 1988; Werner et al. 2004). Seasonal changes to soil water content can increase or decrease air-filled pore space and influence the development of soil fractures. Both features mediate soil tortuosity and exert controls on the soil gas diffusivity rate (Buckingham 1904; Millington and Quirk 1961; Moldrup et al. 1999; Penman 1940; Troeh et al. 1982).

Each texture was represented numerically in the model with a porosity value () from 0-1 based on total air-filled pore space when dry. The textures we tested were: (1) Inorganic clay (= 0.40), (2) silty and sandy clay (= 0.51), and (3) silty sand (= 0.55) (Hough 1966; Terzaghi et al. 1996; Swiss Standard 1999; Truty and Obrzud 2015). To simplify, these soil textures were referred to in the manuscript as clay (= 0.40), loam ( = 0.51) and sand (= 0.55).

We used the porosity of each soil texture to approximate soil gas diffusivity rate () using the modified Millington-Quirk relationship (McCarthy and Johnson, 1995; Millington and Quirk, 1961; Nickerson and Risk, 2009), which is derived from the rate of CH4 diffusion in media with porosity , compared to diffusion in free air and free water:

(4)

where is total soil porosity, is water-filled pore space, and are the diffusion coefficients for CH4 in free water and air, respectively, and H is the solubility constant (Henry’s) for CH4 in water equal to 0.0014.

The CH4 leak (*LR*) represented migrating gas from a compromised wellbore which had infiltrated the uppermost part of the soil column. We modeled CH4 entering (flux-in) at a constant rate of 0.0, 0.1, 0.5, 1.0, 10.0, 50.0 m3 CH4 day-1. In the manuscript, we presented results from the 0.1 and 1.0 m3 CH4 day-1 scenarios to show a 1 order of magnitude difference in rate of gas entering the profile.

**STEADY STATE HOMOGENEOUS AND NON-HOMGENEOUS SCENARIOS**

Diagram, engineering drawing

Description automatically generated

**SI, Figure 1:**

**(A)** Initial conditions for homogenous steady-state scenarios. Initial CH4 concentration (), soil gas diffusivity rate () and porosity () are uniform throughout 10 layers of a 1 m deep soil profile. **(B)** Initial conditions for non-homogenous, steady state scenarios reflecting variation in soil gas diffusivity, porosity, and microbial production of CH4 with depth.

Model results under steady state conditions were output when equilibrium was reached (e.g., ‘flux in’ is equal to ‘flux out’). Under homogenous scenarios the soil profile was uniform, and all parameters were constant. For non-homogenous scenarios, soil parameters varied with depth. Three *DR*, 10-5, 10-6, and 10-7 (m2 s-1) were used to represent sand, loam, and clay textured soils respectively, were applied to both homogeneous and non-homogeneous steady-state scenarios. Under homogenous scenarios, represented soil texture, whereas under non-homogenous scenarios, reflected the effects of compaction, texture, and soil layering.

**TRANSIENT CONDITIONS**

Transient conditions better represent the real-world variability of soil conditions. We assessed five unique Alberta ecoregions: Mixed Grasslands (MG), Moist Mixed Grasslands (MMG), Fescue Grasslands (FG), Boreal Transition (BT), Peace Lowlands (PL). The ecoregions range from dry temperate to boreal climate conditions and represent the range of environmental variability that can occur at a given well site in Alberta, Canada (Downing and Pettapiece 2006). We used two parameters to simulate each ecoregion and defined these two parameters as *soil environmental conditions*: (1) the soil water content (, which is characterized by varying pore space through time to reflect the annual precipitation of each ecoregion, and (2) the variation of microbial CH4 production as a function of temperature (), which was used to reflect daily and yearly temperature variations.

The potential water content within the soil is constrained by total air-filled porosity. Recall that we defined our three soil textures based on their porosity. These values were then applied to each of the five Alberta ecoregions:

The variation in can be described by the following equation:

(5)

where , defined as a fractional unit, is the variation of pore space, is the initial porosity of the soil in units of percent (%), and is the time frame that varies ( defining the initial start time.

Microbial activity () is strongly coupled to temperature and moisture content (Davidson et al. 2006; Lloyd and Taylor 1994; Pumpanen and Hari 2003). As temperature and moisture content increase, the amount of microbial CH4 production also tends to rise (Lloyd and Taylor 1994). Therefore, not only describes diel and annual variation of biological CH4 production, but also the ecoregion’s temperature change. Microbial activity of an ecoregion is defined by the following:

(6)

where is the variability of biological CH4 production in accordance to yearly or daily time frames (µmol m2 s-1), is the biological CH4 that is known to occur on average for the specific ecoregion (µmol m2 s-1), is the time frame that the variation in production occurs in seconds (s) at , is biological CH4 production that occurs within an eco-region over diurnal and seasonal timeframes (µmol m-2 s-1).

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