

Modeling Microbial Oxidation of Organic Compounds by Surface Collision Effects Compared to Kinetic Mechanisms

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Introduction

Landfills have been cited as a primary anthropogenic source of methane to the atmosphere. However, current emission models do not address the complexity of methane oxidation and the attenuating effect that this can have on emissions of methane through the landfill cover. Prediction of landfill emissions on a country basis has remained focused on the quantity of refuse in place versus accounting for interactions within the landfill cover. Field and laboratory studies have shown that the landfill cover itself can oxidize a few percent to all of the methane passing through the landfill cover soils with temperature and soil moisture as primary controlling variables (Boeckx et al., 1996; Whalen et al., 1990). The diffusion of gases into and through the soil is more rapid through air voids than through water films. However, the difficulty is the factors influencing the gas emission and oxidation are extremely site specific (Meadows, 1996). Commonly the microbial oxidation is handled through first order relationships in computational models (Kjeldson and Christensen, 2001). A better understanding is needed in the mechanisms to achieve an accurate model representation of the attenuating effect. Currently methane oxidation can be estimated from the transformation of added $^{14}\text{CH}_4$, the fractionation of natural methane ^{13}C , and the mass balance modeling of concentration gradients (Bastviken, et al. 2002).

Current Research

The initial emission model that was developed (Landfill Methane Emission Model :LMEM) modeled oxidation through a collision algorithm rather than through first order degradation or Michaelson/Menton kinetics. The framework of LMEM allows for the modeling of the predicted maximum oxidation zone and can illustrate some of the limiting factors to methane oxidation (oxygen diffusion and growth media) and has provided a good starting point. Recent work has focused on modifying this model to have a more realistic surface area to volume ratio for the soil particles. Currently all the soil in a node is represented by a single sphere. Therefore, the ratio of surface area to volume for a 1cm^3 node is $\frac{1}{3}(1-\phi)$, where ϕ is the total porosity. For real soils values are several orders of magnitudes higher with the clay soils having surface/volume ratios approaching $10^6\text{ cm}^2/\text{cm}^3$ or higher. This emphasizes the need to increase this ratio in the model. Additional geometric shapes to increase the surface area to volume ratio have also been attempted. Results of this has had limited success due to the complexity of mapping the collision surfaces in the nodes.

Additional efforts have also been made in the modifications to a calibrated heat and gaseous transport model (CHAIN-2D: Simunek and van Genuchten, 1994) to account for the microbial oxidation both kinetically and through soil collision parameters. The advantage of this approach is that both heat and water transport are modeled, so the effects of temperature and moisture on the oxidation rate can be examined. Results of the recent modeling on the effect of the oxidation on soil pH will also be presented as another potential limiting factor to methane oxidation.

Another emphasis has been on determining if an empirical model can be developed from microbial biomass determinations (Jenkinson and Powlson, 1976). This would provide some site specific data that is needed in order to accurately model oxidation. However, due to the complexity of the microbial populations this approach could be extremely limited. The microbial biomass numbers have shown initial promise in laboratory degradation studies.

References

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