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APPLICABILITY OF HEAT AND GAS TRANS- PORT MODELS IN BIOCOVER DESIGN BASED ON A CASE STUDY FROM DENMARK

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SUMMARY: Biocovers — layers of mature compost — can oxidise a considerable amount of methane emitted from landfi Different factors can affect oxidation, particularly tempera- ture. For better understanding of the processes and for future biocover designs, two models (analytic and numerical) were developed. Both models used the heat equation for heat transfer, and the numerical model used advection-diffusion model with dual Monod kinetics for gas transport. The results were validated with data from a Danish landfi The models correlated well with the observed data: the coefficient of determination (R2) was 0.95 for the analytic model and 0.91 for the numerical model. The models can be used for different design scenarios (e.g. varying methane infl thickness or start of operation), and can also help understand the processes that take place in the system, e.g. how oxygen penetration depends on ambient temperatures.

1. INTRODUCTION

The waste management system accounts today for a fourth of total emissions of methane (CH4) from anthropogenic sources (Stocker et al., 2013); high methane concentrations can locally increase explosion risks (Scheutz et al., 2009). Globally, the gas contributes to climate changes and its Global Warming Potential is estimated to be 30 times higher than carbon dioxide's (CO2) (Stocker et al., 2013). One of the biggest contributors from the waste sector are landfills.

Some of the common techniques to minimise methane emissions from landfills involve gas collection systems, but those cannot be applied everywhere; for old and small landfills as well as sites with low organic content use of such technology cannot be economically justified. In such cases biomitigation systems (e.g. biocovers) can be a viable alternative, as successfully shown in three studies at Danish landfi in Fakse, Klintholm and AV Miljø (Nielsen, 2015).

Biocovers are layers of mature compost with active population of bacteria which can oxidise methane to carbon dioxide (methane oxidation, MO) according to the following exothermic reaction (Scheutz et al., 2009):

$$CH4 + 2O2 \longrightarrow 2H2O + CO2 + \text{biomass},\ \Delta G0 = -780\ \text{kJ/mol CH4}. \qquad (1)$$

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Yet another important reaction in the biocover is compost respiration (CR); the organic carbon still present in compost will compete with methane oxidising bacteria for oxygen. In terms of energy budget, both reactions are comparable: the energy released per mole of oxygen is 423 kJ for compost respiration and 390 kJ for methane oxidation (Nielsen, 2015). The energy released in the processes will affect the temperature inside the biocover, which optimally should remain above 40 °C to ensure highest microbial activity (Scheutz et al., 2013). Even though there are other factors affecting biocover's performance (e.g. inhibitors or thickness), the temperature is a necessary condition for the biocover to work.

Therefore, especially in colder climates, it is important to incorporate heat transfer models at the design stage.

Mathematical models for biocover designs have been available for over a decade, yet to the best of our knowledge, none of them couples temperature with gas transport and at the same time use varying boundary conditions and field data. Neither do they include effect of compost respiration on both the temperature and the amount of available oxygen. Some of the early models were only validated by laboratory experiments (De Visscher and Van Cleemput, 2003). Other used a combination of field data and constant environmental conditions, or tried to develop correction factors for the reaction rates to account for non- homogeneous field conditions (Abichou et al., 2011). The only model known to authors which couples heat and gas transport is only validated using a simple soil experiment from an earlier study (Ng et al., 2015). Analytic models suffer from the same simplistic approach; even the latest work by Yao et al. (2015) does not include temperature development and is only validated using one laboratory experiment.

This work hopes to fill this gap; the objective is to present two one–dimensional models and to analyse the results in terms of their applicability for a biocover design, as well as their accuracy in predicting the observed field data. Both the analytic model with energy term varying with depth and numerical model built with COMSOL Multiphysics v.4.4 have temperature dependence and hence can be used to model seasonal changes and as a filtering method for appropriate designs. The numerical model couples both temperature, methane and oxygen concentrations and includes the effect of compost respiration. Finally, the models were validated with field observations from the AV Miljø landfi

2. METHODS

2.1 Field description and general assumptions

The biocover system at AV Miljø landfi in Copenhagen consisted of two layers: gravel gas distribution layer with active pumping system (about 40 cm thick) and layer of compost (about 90 cm thick). The total area of the biocover was 400 m2. Two water locks were installed to close possible lateral escape paths, and a riffled interface between the layers was adopted to avoid water buildup. Unlike the usual setup, the biocover system was placed over the existing top cover and it was fed by dilute landfi gas pumped out of the adjacent leachate wells. The total pump rate and gas composition were measured to control the gas load to the biocover. The diluted landfi gas was mixed with atmospheric air (Kjeldsen et al., 2013).

Measurements on-site confirmed a very homogeneous gas distribution in the East–West cross-sections, whereas the southern regions of the biocover were generally supplied with higher gas infl (Kjeldsen et al., 2013). As the horizontal extent of the biocover was large compared to its depth, a one–dimensional model is sufficient despite a non–homogeneous gas distribution in the North–East direction. In both models it is assumed no heat exchange occurs with the gas distribution layer (Neumann boundary condition at the bottom), whereas the temperature on the surface is known

(Dirichlet boundary condition at the top). Most importantly, the water content inside the biocover is assumed to be constant.

2.2 Analytic model

The governing equation in the analytic model is the heat equation

$$c_m \rho \frac{\partial u}{\partial t} - K \frac{\partial^2 u}{\partial x^2} = S(t, x) \tag{2}$$

where c_m is the specific heat capacity, ρ is soil density, K is thermal conductivity, u is temperature and $S(t, x)$ is a time and depth dependent function describing energy generation inside of the biocover as a result of methane oxidation and compost respiration.

From the biological perspective the function $S(t, x)$ should attain maximum around depth of 20–30 cm, where the optimal temperature and oxygen conditions are found (Scheutz et al., 2009). From a modelling perspective this function should be smooth and preferably easy to integrate. In the model the energy function is defined as $S(t, x) = -S_{amp} \cos(2\pi x) + S_{mean}$, where S_{mean} and S_{amp} are the mean energy generation inside the biocover and the fluctuation from the mean. The estimates of the energy generation come from the average methane influx and the energy from oxidation per mole of methane. The choice of a cosine function follows from its desirable properties: it is generally easy to integrate, and by making one of the variables redundant (no time dependence), the calculations can be further simplified. Lastly, it attains a maximum at x = 45 cm, which is an acceptable simplified. The solution is derived from eigenfunctions and Fourier series for heat equation, where by using method of shifting data a non-homogeneous boundary value problem can be expressed as a sum of a solution to a homogeneous boundary value problem uh(t, x) and an auxiliary function $u_a(t, x)$, such that $u(t, x) = u_h(t, x) + u_a(t, x)$:

$$u_a(t, x) = \left(1 + \alpha\left(x - \frac{x^2}{2L}\right)\right) T_s(t) \tag{3}$$

$$u_h(t, x) = \sum_{n=1}^{\infty} \left(\tilde{\phi}_n \mathrm{e}^{-C_1 m^2 t} + \int_0^t \mathrm{e}^{C_1 m^2 (s-t)} \tilde{S}_n(s) \mathrm{d}s \right) \beta \sin(mx) \tag{4}$$

$$\tilde{\phi}_n = -\frac{2}{L} \int_0^L \alpha \left(x - \frac{x^2}{2L}\right) T_s(0) \sin(mx) \mathrm{d}x \tag{5}$$

$$\tilde{S}_n(t) = \frac{2}{L} \int_0^L \left\{ S(t, x) - \left(1 + \alpha\left(x - \frac{x^2}{2L}\right)\right) T_s'(t) - \frac{1}{L} T_s(t) \right\} \sin(mx) \mathrm{d}x \tag{6}$$

where L is the depth of the biocover, $T_s(t)$ is the surface temperature function, $C_1 = K/(\rho c_m)$, $m = (2n + 1)\pi/(2L)$, and α, β are empirically found correction factors. Values of all parameters are presented in Table 1.

2.3 Numerical model

The numerical model has three governing equations: heat equation for temperature, $u(t, x)$, where the energy term consists of the methane oxidation and compost respiration compo- nents; equations for methane and oxygen concentration ($M(t, x)$ and $O(t, x)$) where dual Monod kinetics accounts for the gas consumption due to methane oxidation and which as- sume diffusion as the only transport process. The equations are:

$$c_m\rho\frac{\partial u}{\partial t} = K\frac{\partial^2 u}{\partial x^2} + CR(u,O) + \min\left\{\frac{V^m_{max}\cdot M}{K^m_h + M};\frac{1}{\beta_o}\frac{V^o_{max}\cdot O}{K^o_h + O}\right\}\frac{E_{ox}B}{M_w} \tag{7}$$

$$\frac{\partial M}{\partial t} = D_{\text{diff}}\frac{\partial^2 M}{\partial x^2} - \min\left\{\frac{V^m_{max}\cdot M}{K^m_h + M};\frac{1}{4}\frac{V^o_{max}\cdot O}{K^o_h + O}\right\}B \tag{8}$$

$$\frac{\partial O}{\partial t} = D_{\text{diff}}\frac{\partial^2 O}{\partial x^2} - \left(\min\left\{\frac{4V^m_{max}\cdot M}{K^m_h + M};\frac{V^o_{max}\cdot O}{K^o_h + O}\right\}B + CR^o(u)\right) \tag{9}$$

where $CR^o(u)$ is a temperature and oxygen dependent function which expresses oxygen consumption due to compost respiration (the function is interpolated from the data from Scheutz et al. (2013)), $CR(u, O)$ is the energy generated through compost respiration, whereas the remaining parameters are explained in Table 1.

The boundary conditions for u are identical to the analytic model, whereas for methane and oxygen the concentrations on the surface are assumed to be constant (and equal to atmospheric concentrations), whereas the fluxes at the bottom are equal to the measured fluxes on-site.

Table 1. Parameter values used in the models (detailed information, including sources, can be found in Nielsen (2015)).

Parameter	Symbol	Value	Unit
Biocover			
specific heat capacity	c_m	1.02	[J/(K · g)]
compost density	ρ	505	[kg DM/m^3]
thermal conductivity	K	0.27	[J/(s · m · K)]
total porosity	θ	0.75	[–]
air-filled porosity	θ_a	0.37	[–]
depth	L	0.9	[m]
microbial population	B	0.9	[kg/m^3]
Gas properties			
diffusion coeff., CH_4–O_2, 20.5 °C	D_0	0.215	[cm^2/s]
effective diffusion coeff., CH_4–O_2	D_{diff}	0.03	[cm^2/s]
average uptake coefficient, methane	V^m_{max}	2.11	[µmol/(h · g)]
half saturation constant, methane	K^m_h	15.1	[µmol/L]
energy from methane oxidation	E^m_{ox}	780	[kJ/mol]
methane emissions	Em	15	[kg CH_4/day]
maximum specific uptake, oxygen	V^o_{max}	1.37	[µmol/(h · g)]
half saturation constant, oxygen	K^o_h	58	[µmol/L]
oxycaloric coefficient	E^o_{ox}	423	[kJ/mol]
Analytic model			
correction factor 1	α	0.3	[–]
correction factor 2	β	0.06	[–]
mean energy generation	S_{mean}	2.3	[K/day]
fluctuation of energy generation	S_{amp}	1.26	[K/day]

3. RESULTS AND DISCUSSION

3.1 Validation with measurements on-site

The models are validated using temperature measurements from different depths inside the biocover at AV Miljø. The comparison of the modelled and measured data is presented in Figure 1. The colours correspond to different times at which the measurements were taken, where red corresponds to the beginning of the monitoring period (September 2012) and blue to the end of that period (January 2013). Ideally, the temperature monitoring should take place for at least one year to account for warmest and coldest temperatures in a year. In this case, however, it is acceptable that only the colder months are considered, as temperature should not be limiting during summer and spring.

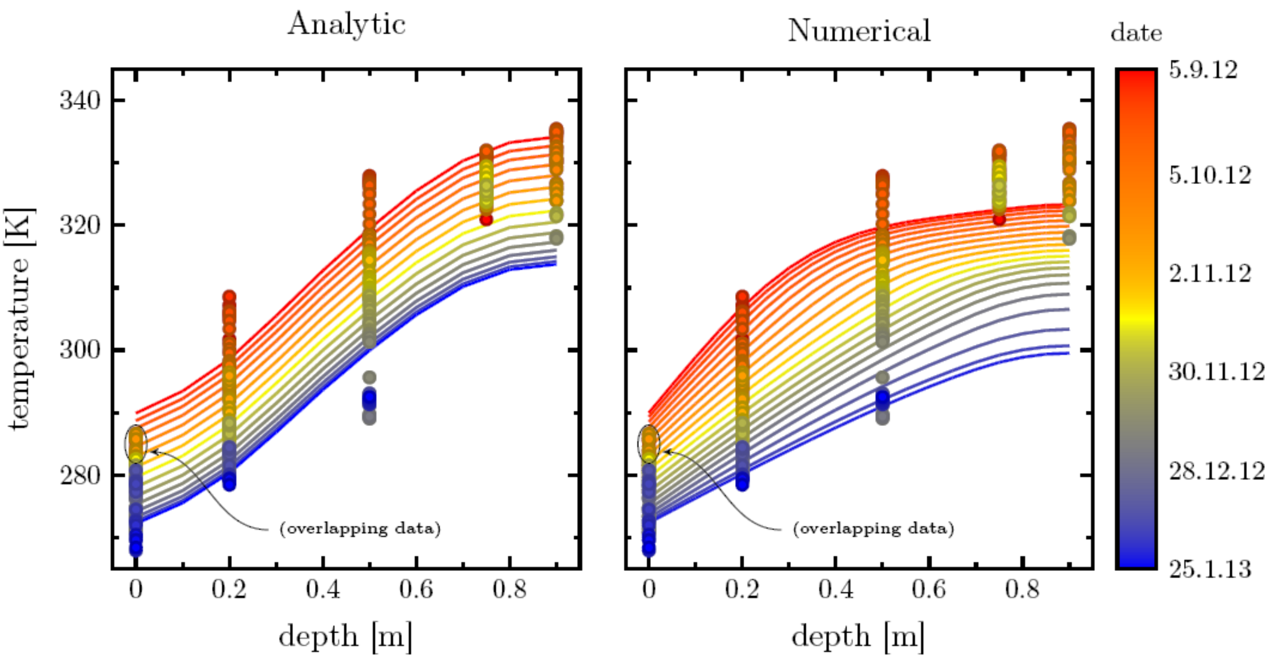

Figure 1. Modelled temperature (solid lines) and observed temperature (dots) for the two models.

Both models, despite representing different temperature developments, fit very well to the observed data. The coefficient of determination (R^2) is very high; the value reaches 0.95 for the analytic model and 0.91 for the numerical model (value equal to 1 corresponds to a perfect fit).

At the same time, the results illustrate different temperature regimes for which the models are most accurate; the analytic model predicted very well higher temperature ranges at the bottom of the biocover, whereas the numerical model was superior in predicting lower temperatures. That property is particularly useful when assessing biocover performance in colder climates, where lower temperatures can easily become limiting.

3.2 Oxygen–limiting conditions

Temperature profiles in the numerical model reach a plateau in the deeper 40 cm of the bio- cover ($0.5 \leq x \leq 0.9$) in the beginning of the monitoring period (September/October 2012). The measurements seem to reach a similar plateau around the same depth, although the actual temperature is higher than predicted. This stagnation is a consequence of oxygen- limiting conditions; high ambient temperature allows theoretically for a high microbial up- take rate of methane, yet this rate is inhibited by low oxygen concentrations in the pore spaces.

Too little oxygen in the deeper parts of the biocover is a common design problem, as oxygen diffusion is often slower than oxidation rate. This usually results in a limited oxygen penetration into the oxidising layer. At AV Miljø landfill gas was mixed with atmospheric air (the gas collection system from the leachate wells was not airtight), and this was expected to influence the oxidation close to the bottom boundary. Indeed, by modelling two scenarios with identical methane influx, but varying oxygen influx (no influx in one case, and the influx from AV Miljø in the second case), different methane oxidation efficiency was obtained for each case; 85% of methane was oxidised when there was no oxygen bottom flux, whereas the efficiency increased to 94% if oxygen was part of the pumped gas mixture. Moreover, the emission peaks coincide in both cases with higher peaks in the case where no oxygen was pumped into the biocover. With or without oxygen bottom flux surface oxygen was able to diffuse at least to a depth of 50 cm, and on colder days even deeper (results not shown); as specific uptake rate of methane (and thus the oxidation rate) is temperature dependent, lower ambient temperature lowers this rate and hence there is a potential of deeper oxygen penetration, as not all gas is depleted in the upper parts of the biocover.

3.3 Start of operation

Good biocover performance from the first day of operation requires a careful investigation of the local climate. To illustrate this issue, two scenarios have been modelled: one starting January 1, whereas the other starting June 1 (both models had identical bottom fluxes). The results are unambiguous: while the biocover performs well immediately after installation in the June scenario, it requires almost 5 months to increase the temperature to a suitable level for the January scenario (the temperature throughout the biocover is equal to the ambient temperature in the initial period, Figure 2).

The theoretical 5-month delay for microbial activity to start in reality could mean death of the entire community. In the model microbial community is assumed to be constant throughout the biocover and through time. In reality, however, the community will be highly affected by the lower temperatures and in that respect installing the biocover in the early summer, rather than spring or winter can become single–handedly the most important factor affecting biocover performance.

3.4 Predictive capabilities

In every model there needs to be a balance between complexity and accuracy on one hand and flexibility on the other. The two models presented in this paper are capable of predicting correct trends as exemplified by Figure 1, while remaining relatively simple. The simplicity is important: first of all, it ensures transparency, which is necessary for the models to be used by non-modellers. Second of all, it ensures flexibility, as the models can easily be adapted to various climates and conditions. By combining analytic and numerical models, one can obtain a more in-depth understanding of the processes at stake, as these two modelling approaches have complementary strengths and different limitations.

Analytic model is very easy to understand and fairly straightforward to implement; the only non-trivial element in this model is the energy generation function $S(t, x)$. This can be adjusted to particular needs: by shifting the maximum of the cosine function one can freely define the oxidation front (i.e. the depth at which energy generation peaks); time dependence can be included; other non-trigonometric functions can be used if particular data set suggests it is more suitable. In short, any smooth function is applicable depending on the particular case studies.

The biggest limitation of the analytic model is its incapability of tracking methane and oxygen concentrations. For that reason analytic model is very useful in the initial design stage as it can determine whether temperature can potentially be a limiting factor, yet is not enough to predict actual oxidation efficiency.

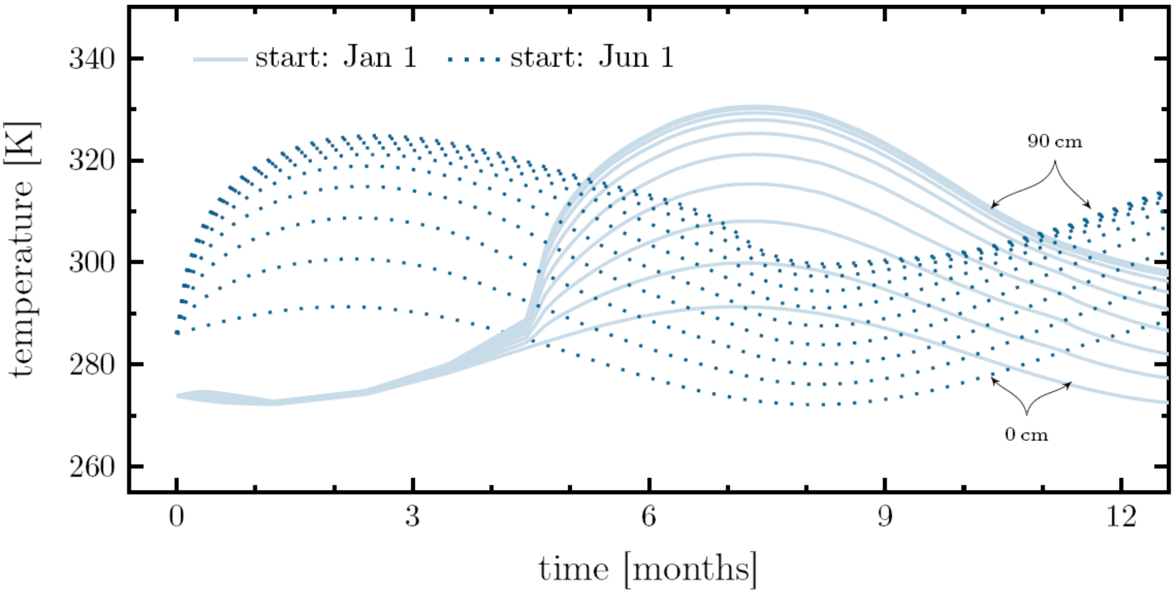

Figure 2. The effect of ambient temperature on the temperature development in the first year. The lines correspond to x = {0, 10, ..., 90} and the temperature increase gradually.

For that purpose the numerical model is an excellent tool; it allows for complicated problem formulations for which exact solutions almost certainly do not exist. Moreover, it can model complicated boundary conditions and multiple parameter dependencies can be included (for instance, thermal conductivity depends on water content, which depends on precipitation).

On the other hand though, the current version of the model has two important limi- tations. First of all, water content is assumed to be constant in time and space, whereas previous studies have shown that moisture content in soil will be affected by precipitation (soil response will vary depending on depth: moisture in the deeper layers will fluctuate more, (Nielsen, 2015)), or water produced during the oxidation process (Ng et al., 2015).

Second of all, only two gases are included in the model, which allows for a simpler advection–diffusion model to be used. If more gases were considered (nitrogen and carbon dioxide in particular), a different formulation of the problem is necessary, as the Fickian ap- proach fails for multiple gas mixtures and Stefan–Maxwell equations should be used instead.

Useful models are not those which are 100% accurate, but rather those that — despite their limitations — can account for various design scenarios. In case of the models presented here the applicability range is wide: increased methane influx; varying thickness of the biocover; contribution of compost respiration to the total energy budget; correct installation time and others. Furthermore, with some adjustments the models can also account for varying microbial community and effect of moisture content on oxidation efficiency.

4. CONCLUSIONS

Two models — analytic and numerical — were developed to accurately describe temperature development due to methane oxidation and compost respiration in a biocover system at the AV

Miljø landfi in Copenhagen. Both models used the heat equation as the governing equa- tion for temperature. Moreover, the numerical model coupled temperature with methane and oxygen concentrations via dual Monod kinetics.

High values of the coefficient of determination (R2) confirm that both models can accurately describe heat transfer in biocover and even with a number of simplifications (constant microbial population, constant water content in porous medium), the models are suitable for biocover design. Simplicity of the formulation ensures flexibility in assessing different scenarios (start of operation, varying bottom methane flux, biocover thickness, contribution of compost respiration to the total energy budget). The models can also help understand the processes taking place inside the biocover, such as oxygen penetration as a function of temperature (for colder days, the penetration is deeper).

Analytic and numerical models have different characteristics from which follow different strengths and weakness. Analytic models tend to be more transparent and easier to un- derstand by non-modellers. At the same time the energy generation function used in the analytic model (S(t, x)) gives freedom to model the processes as complicated as possible given the knowledge of the particular biocover system. Provided the function is smooth, it should not have any consequences on the calculation time or existence of the solution.

The analytic model can only be used for preliminary results; it can indicate temperature– limiting conditions, but not the actual oxidation efficiency. For that purpose the numerical model is more suitable. By adjusting boundary conditions different scenarios can be simu- lated and efficiency estimated. The model can be improved by adjusting moisture content in the pores, which is affected by both rainfall and water generated during methane oxidation.

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