SIMULATIONS OF MIGRATION AND EMISSIONS OF GASES IN SAND-COVER OF LANDFILL.

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ABSTRACT

The migrations and emissions of landfill gases in porous sand cover can be estimated with empirical correlations and simulated with a computing fluid dynamics (CFD) scheme. The sand-covers of 0.3 m and 0.6 m are treated as porous media. The CFD simulations are particularly useful in capturing the mechanism of migration and emissions of gases under steady and unsteady-state conditions. It is found that the mass transfer may be driven by simultaneous diffusion and buoyancy convection. The rate of mass transfer is significantly enhanced compared to that of diffusion, generally it is about three times that of pure diffusion. The prediction of mass transfer rate by diffusion of gas in stationary fluid in porous media is found to be lower than the prediction from CFD simulation. The CFD simulations can also be designed to predict the level of emissions which must meet regularly standard of health and safety.

Keywords: *emissions of gases, convection, porous media, CFD simulations.*

1.0 INTRODUCTION

Landfill gas consists mainly of carbon dioxide and methane is produced during the degradation of the organic wastes by microorganisms. The concentration gradient created will lead to gas diffusion, where the gas will migrate either vertically to the atmosphere or laterally beyond the landfill boundaries. Aside from the gas diffusion, natural convection occurs due to the adverse density gradient (Rayleigh, 1916), which may enhance the migration of the gases.

Methane is a greenhouse gas. Furthermore, it is an explosive gas when its volumetric concentration attains 5 to 15% in the air mixture. Due to safety reasons, a very careful control for the gas emissions at landfills is required. Another incentive for controlling the methane gas is that it is a valuable energy source.

Farquhar (1987) had conducted numerical simulations of gas migration beyond lateral landfill boundaries. While other researchers such as Lang and Tchobanoglus (1989) simulated the gas generation and migration within the landfill only. Nevertheless, less attention has been devoted to the effect of the convection on the gas migration. This study aims to provide a better simulation for the onset of convection in landfill gas migration process.

2.0 TRANSIENT RAYLEIGH NUMBER FOR NATURAL CONVECTION

The most important criterion for the onset of instability for porous media is the critical Rayleigh number,

$$Ra = \left(z^2 K_e g / m D_{eff}\right)\left(\partial r / \partial z\right) \quad (1)$$

where D_{eff} is the effective diffusion coefficient across the porous media. The key equations are adopted from the transient instability theory of Tan *et al.* (2003) for the prediction of the onset of convection caused by mass diffusion in porous media. They proposed the concept of maximum local density gradient, $\partial r / \partial z$ and maximum penetration depth, $z_{\max}$ which are controlled by the boundary condition of the system. The gas-gas diffusion system tends to a Biot number $Bi = \sqrt{D_1 / D_2}$ of approximately one, which corresponds to the constant mass flux (CMF) boundary condition.

Crank (1975) showed that the corresponding concentration profile at CMF boundary condition is given as: $(c_0 - c_1) = \left(2 j \sqrt{D_{eff} t} / D_{eff}\right) ierfc\left(z / 2\sqrt{D_{eff} t}\right)$. Applying the mathematical principle advanced by Tan and Thorpe (1996), the maximum local density gradient is defined as: $(\partial c / \partial z)_t = -\left(j / D_{eff}\right) erfc\left[z / \left(2\sqrt{D_{eff} t}\right)\right]$. The maximum transient Ra_c for CMF may be derived at $z_{\max} = 1.684\sqrt{D_{eff} t}$ as:

$$Ra = \left(0.6634 t K_e g j\right) / \left(D_{eff}\, m\right) \quad (2)$$

For bottom-up diffusion with a top free surface, the theoretical critical value of Ra is found to be 27.1 (Nield, 1968 and Rabando and Torrance, 1976). For Ra equal to 27.1, the corresponding critical time is:

$$t = \left(40.85 m D_{eff}\right) / \left(K_e g j\right) \quad (3)$$

There are many ways to define the D_{eff}. In this study two different D_{eff} were examined. According to Satterfield (1970), the D_{eff} in a porous media is defined as below:

$$D_{eff}{*} = De / t \quad (4)$$

where e is equal to the void fraction of the porous media, t is the tortuosity and D is simply the diffusion coefficient of the gas without porous media. Due to the inherent structure of the porous media model of the FLUENT, t will be equal to 1, then Equation (5) will be reduced to $D_{eff}{*} = De$.

Maxwell (1873) considered the effect of the diffusion into the solids and defined the D_{eff} of a porous media as:

$$D_{eff}^{\#} / D = \left(1 + 2e_s\right) / \left(1 - e_s\right) \quad (5)$$

if the diffusion of the gas into solid is insignificant. ε_S is the volume fraction of the spheres, which is equal to 1-ε. It should be noted that both definitions for D_{eff} are independent of the diameter of the particles.

3.0 CFD SIMULATIONS

A CFD package, FLUENT was used to simulate the migration of landfill gas. CH_4 was chosen as the landfill gas in the simulations. The sand will be assumed to have a uniform size which forms a homogenous sand cover. In the simulations, the porous sand bed was represented by a rectangular domain with an open top, which serves as a free surface. The porous medium initially was saturated with air at 1 atm. and 282 K as shown in Figure 1.

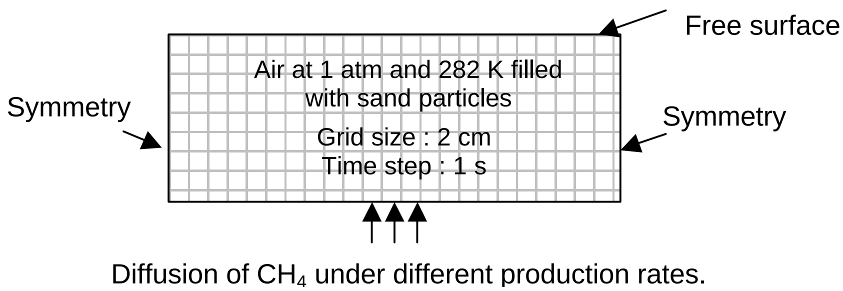


Figure 1: Configuration of the porous sand bed for simulations.

Three different particle diameters, 0.003, 0.0045 and 0.006 m were used to study the effects of permeability on the gas migration. Similar to the particle diameters, three different porosities, 0.255 0.355 and 0.455 were applied in the simulations. The combination of the different particle size with different porosity will yield a range of permeability of the sand bed where the effect of the permeability to the gas migration can be show very clearly. Miroslav *et al.* (2000) used a constant rate production rate of 3.3 kg/t/yr of CH_4 in their modeling. In this study, the CH_4 assumed to be emitted from the bottom of the bed at a constant rate production at 1.00 x 10^{-4} m^3/s.

The time step was set at 1 second, which should be small enough to yield accurate simulations since the critical time was found to be in the range of 50 to 200 second from analytical solution. Holman (2001) noted that over refined grid sizes tend to generate inaccurate results due to the cumulative numerical round-off error. The grid size of each case of simulation was optimized and refined to generate acceptable accuracy with reasonable computing expenses. The setting of the various cases was shown in Table 1.

Table 1: Settings of the various cases of simulation

Case	Particle diameter, m	Porosity	Permeability, x 10^8 m^2	D_{eff}*, x 10^6 m^2/s	$D_{eff}^{\#}$, x 10^6 m^2/s	Domain size, m x m
1	0.0060	0.355	2.24	7.15	5.41	1.15 x 1.15
2	0.0060	0.455	6.61	9.16	7.20	0.70 x 0.70
3	0.0030	0.455	1.65	9.16	7.20	1.15 x 1.15
4	0.0030	0.355	0.56	7.15	5.41	2.30 x 2.30
5	0.0060	0.255	0.62	5.14	3.74	1.27 x 1.27
6	0.0045	0.455	3.72	9.16	7.20	1.00 x 1.00
7	0.0045	0.355	1.26	7.15	5.41	1.23 x 1.23
8	0.0045	0.255	0.35	5.14	3.74	2.56 x 2.56

Production rate = 0.0001 kg/m^2.s at 282 K, 1 atm., time step = 1 s.

3.1 CONTROL CASES

Control cases were simulated to provide evidence that the convection effect is not due to any numerical effects or errors, such as numerical diffusion. In control cases, the air served as the source, which was diffused into the porous media pre-saturated with CH_4. For buoyancy convection to occur, an adverse density gradient must be developed (Lord Rayleigh, 1916). It is expected that natural convection will not occur, as shown in Figure 2, since the adverse density gradient cannot be developed in the control cases. This remains so even after a considerable amount of time exceeding one hour, only uniform density regime was observed. This clearly supports that the occurrence of convection in other simulations is purely caused by the presence of the adverse density gradient.

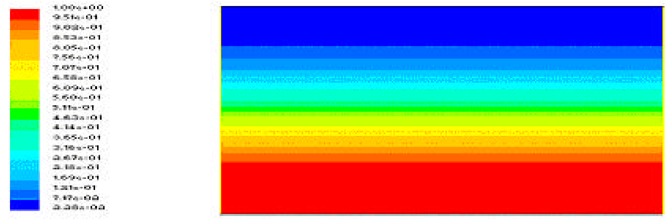


Figure 2: Contours of mass fraction of air diffusing into the porous sand bed pre-saturated with CH_4.

4.0 RESULTS AND DISCUSSION

The results of simulation show that the onset of convection occurs after an initial stable diffusion period. This means that the rate of migration of the CH_4 through the porous media would be enhanced due to natural convection. The convection plumes in the sand bed are in the fingering shape, which is similar to the results of the analogous thermal diffusion of Tan *et al.* (2003).

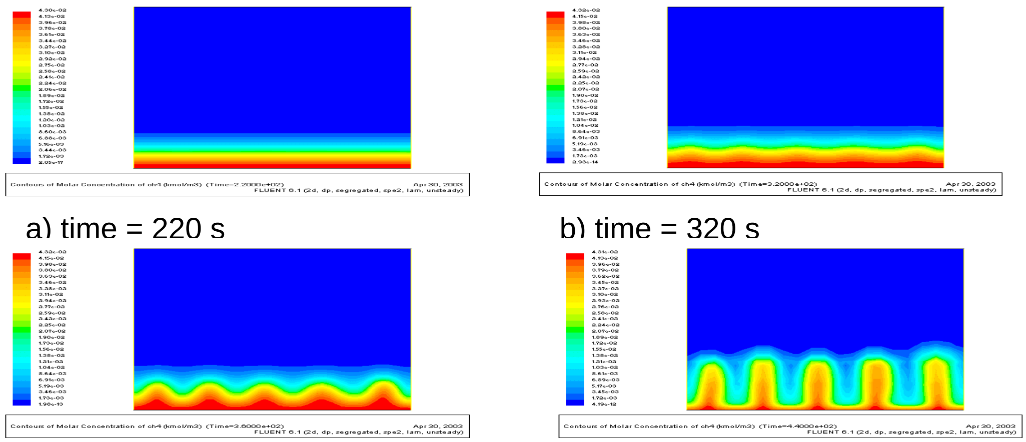
4.1 FORMATION AND DEVELOPMENT OF THE CONVECTION PLUMES.

Initially the CH_4 diffused into the porous media by a combination of mixing and displacement of the air. A quasi-stable regime of the gas mixture was formed at the bottom layer of the porous sand bed. An adverse local density gradient $\partial r / \partial x$ developed steadily at this point as shown Figure 4(a). After the critical time, t_c, the $\partial r / \partial x$ exceeded a critical value at the critical depth that marked the beginning of convection. The fluid layer becomes unstable as shown in Figure 4(b) and 4(c). Filaments of convection plumes first formed and developed into the fingering shape. The fingering plumes then move towards the upper part of the bed, as shown in Figure 4(d). They may merged and formed larger plumes before detachment. It was observed that for higher permeability bed, the fingering convective plumes tend to coalesce into bigger plumes. While at very low permeability bed, the merging of the convective plumes may not happen, since the movement of the plumes is restricted by the sand particles.

4.2 TRANSIENT RAYLEIGH NUMBER

The transient Rayleigh numbers, Ra_c for the simulations were calculated from the properties of CH_4 at 282 K and 1 atm. The known production rate and critical times obtained from the simulations were used to calculate the transient critical Rayleigh number using D_{eff}* and $D_{eff}^{\#}$ respectively. The average critical Ra* based on D_{eff}* is 29.68, which agrees with the theoretical value of 27.1,Table 2. While the average value of $Ra^{\#}$ was 39.8, which is 47% bigger than the theoretical value, 27.1. This shows that Maxwell's (1873) empirical correlation for the effective diffusivity may be not applicable in this case.

The influence of the permeability of the sand cover on the Ra_c is rather insignificant, Figure 5. However it should be noted that for bed permeability less than 1.0 x 10^{-8} m^2, the simulated Ra_c tend to deviated from the predicted Ra_c. This is because the particle bed is so dense that it provides very high resistance against the movement of the gas, it delayed the onset of the convection. Also at low permeability the onset time become very long, which may cause CH_4 to move laterally and saturated the zone near the boundary. This tends to even out the effect of the density gradient, which also delayed the onset of convection.



a) time = 220 s b) time = 320 s

c) time = 360 s d) time = 440 s

Figure 4: Molar fraction of CH_4 for case 3 (permeability = 1.65 x10^{-8} m^2) at different time steps.

Table 2: Comparison of the simulated and theoretical critical Ra.

Case	Permeability, x 10^8 m^2	Theoritical Ra_c	Simulated Ra_c*	Simulated $Ra_c^{\#}$
1	2.24	27.1	19.5	25.8
2	6.61	27.1	17.1	21.8
3	1.65	27.1	25.6	36.3
4	0.56	27.1	44.3	58.6
5	0.62	27.1	30.9	42.4
6	3.72	27.1	28.7	36.5
7	1.26	27.1	28.9	38.8
8	0.35	27.1	42.4	58.2
	Average	27.1	29.68	39.8

* Ra* based on D_{eff}* and $Ra^{\#}$ on $D_{eff}^{\#}$.

4.3 CRITICAL ONSET TIME OF CONVECTION.

The critical times for the onset of convection were obtained by observing the development of the concentration contour and the sudden increase of the maximum velocity of the CH_4. The simulated critical times were compared to Equation (3) by using D_{eff}* and $D_{eff}^{\#}$ respectively. It was found that the simulated critical times were in good agreement with the predicted time by using the D_{eff}* as shown in Table 3. The effect of $D_{eff}^{\#}$ seems to be more significant for higher permeability.

The difference between the simulated and predicted critical time become very big as the bed permeability dropped to less than 1 x 10^{-8} m^2,as shown in case 4 and 5. At this point the simulated critical times were always longer than the predicted time. Very small permeability provided very high resistance to the flow of the CH_4, which delayed the onset of the convection.

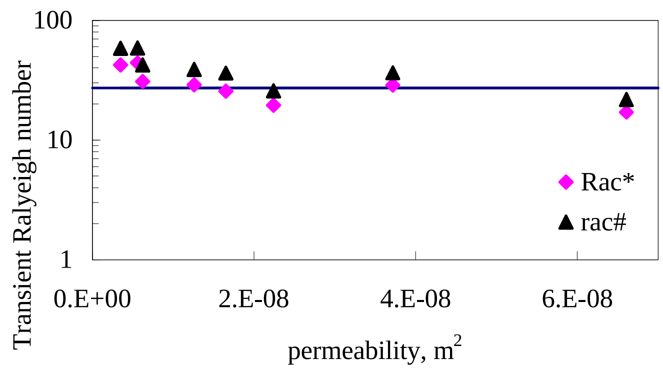


Figure 5: Transient Rayleigh number from simulation for various cases.

Table 3: Comparison of the simulated and predicted critical onset time of convection.

Case	Permeability, x 10^8 m^2	Predicted time, s (D_{eff}*)	($D_{eff}^{\#}$)	Simulated time, s	Difference, % (D_{eff}*)	($D_{eff}^{\#}$)
1	2.24	153	116	110	28	5
2	6.61	66	52	42	36	19
3	1.65	226	209	280	24	34
4	0.56	661	462	1000	51	116
5	0.62	395	288	450	14	56
6	3.72	118	92	125	6	36
7	1.26	270	205	290	7	41
8	0.35	702	511	1100	57	115
				average	28	50

4.5 MAXIMUM VELOCITY OF CH_4.

Upon the onset of convection, the transfer of the CH_4 will be enhanced by a sudden increase of its velocity as shown in Figure 6. During this stage, the velocity of the CH_4 for case 3 shot up from about 0.0002 m/s to 0.006 m/s after the onset of convection, which is about 30 times. The results generally showed that the onset of the convection can increase the velocity by at least 10 times. The influence of the permeability on the sudden increase in CH_4 velocity is very significant. Low bed permeability will yield a smaller increment of the velocity as expected in case 5.

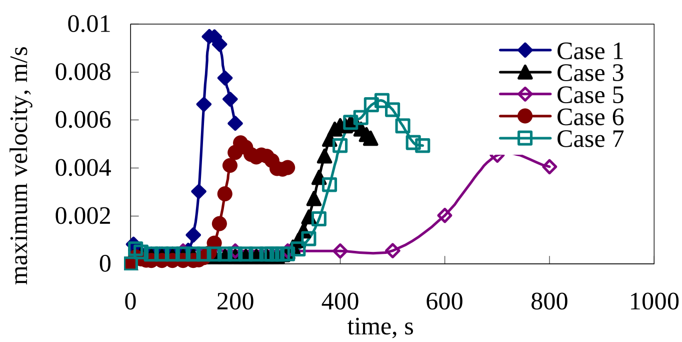


Figure 6: Maximum velocity of CH_4 over time for selected cases

4.6 MASS TRANSFER COEFFICIENT

The instantaneous mass transfer coefficient at the boundary of the porous sand bed shows an initial phase of diffusion that obeys Fick's Law, $j = 0.89\sqrt{D_{eff}^{*}/t}\left(c_s - c_o\right)$ or $j = k_G\left(c_s - c_o\right)$, Figure 7. It started to depart from the theoretical value and stay constant after a brief stable period of diffusion. This is because the surface concentration of CH_4, c_S began to stay constant. From Figure 7, the maximum mass transfer coefficient is about 4 x 10^{-4} m^2/s where the corresponding Sherwood number is about 4 which is comparable with the value of the maximum Nusselt number of 3.4 of Tan *et. al.* (2002) for thermal instability in porous media.

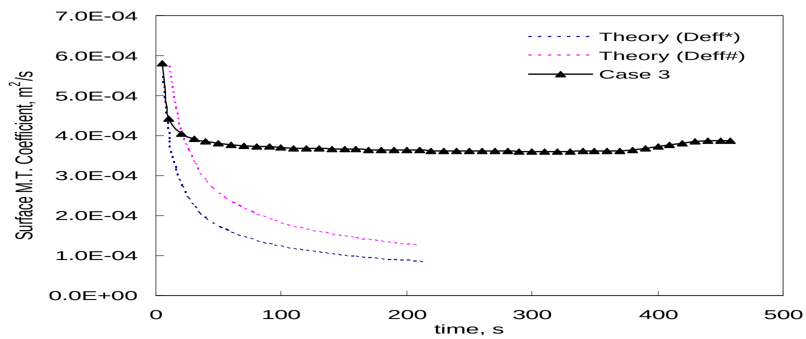


Figure 7: Surface Mass Transfer Coefficient at the Boundary for Case 3.

5.0 CONCLUSIONS

The landfill gas migration in a porous sand bed under CMF boundary condition has been successfully simulated using a CFD package, FLUENT. It shows that the phenomenon is characterized by an initial period of stable diffusion and followed by the onset of convection. Hence the conventional steady-state model with a finite concentration distribution is not very accurate although it is very useful as an analytical solution. The CFD simulation is very useful in providing clear, complete and detailed process of the migration of the landfill gas. They provided very detailed flow field and concentration profiles, which are very difficult to obtain by conducting onsite or offsite measurements. The formation and development of the fingering convection plumes can be distinguished into three different regimes, namely: stable diffusion, onset of instability and convection, and formation of the fingering convection plumes. Upon the onset of convection, the gas migration is enhanced due to the rapid increase in velocity. The maximum Sherwood number is found equal to 4. The critical times from the simulations can be predicted accurately using the transient Rayleigh number developed by Tan *et. al.* (2003). The average critical transient Rayleigh number of the simulations is 30, which is close to the theoretical value 27.1.

NOMENCLATURE

- *c* concentration [kg/m^3]
- *D* diffusion coefficient [m^2/s]
- *g* acceleration due to gravity [m/s^2]
- *j* mass flux [$kg/m^2.s$]
- *t* time [s]
- *z* penetration depth [m]

μ viscosity [Pa.s]
ρ density [kg/m^3]

Abbreviation
CFD computational fluid dynamics
CMF constant mass flux
Ra Rayleigh number

Subscripts
eff effective
s surface
o bulk
max maximum

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