Numerical simulation of landfill aeration using computational fluid dynamics

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Abstract
The present study is an application of Computational Fluid Dynamics (CFD) to the numerical simulation of landfill aeration systems. Specifically, the CFD algorithms provided by the commercial solver ANSYS Fluent 14.0, combined with an in-house source code developed to modify the main solver, were used. The unsaturated multiphase flow of air and liquid phases and the biochemical processes for aerobic biodegradation of the organic fraction of municipal solid waste were simulated taking into consideration their temporal and spatial evolution, as well as complex effects, such as oxygen mass transfer across phases, unsaturated flow effects (capillary suction and unsaturated hydraulic conductivity), temperature variations due to biochemical processes and environmental correction factors for the applied kinetics (Monod and 1st order kinetics). The developed model results were compared with literature experimental data. Also, pilot scale simulations and sensitivity analysis were implemented. Moreover, simulation results of a hypothetical single aeration well were shown, while its zone of influence was estimated using both the pressure and oxygen distribution. Finally, a case study was simulated for a hypothetical landfill aeration system. Both a static (steadily positive or negative relative pressure with time) and a hybrid (following a square wave pattern of positive and negative values of relative pressure with time) scenarios for the aeration wells were examined. The results showed that the present model is capable of simulating landfill aeration and the obtained results were in good agreement with corresponding previous experimental and numerical investigations.

1. Introduction
Landfill aeration is an important effective technology for converting conventional anaerobic landfills into biologically stabilized ones, exhibiting very low emission potential (Ritzkowski and Stegmann, 2012). During the last decades, landfill aeration has been successfully used as a method of landfill remediation worldwide (Heyer et al., 1999, 2003, 2005, 2007, 2009; Ritzkowski and Stegmann, 2005, 2012; Cestaro et al., 2006; Cossu et al., 2007; Ritzkowski et al., 2009a, 2009b). Investigations on landfill aeration were conducted at laboratory as well as pilot and field scale. In practice, the design of field scale aeration systems was based on preliminary pilot scale experiments as well as on previous practical experience (Cestaro et al., 2006). Some computational models were used as auxiliary tools combined with the pilot experiments (Cossu et al., 2007), in order to elucidate parameters, such as the radius of influence of each aeration well.

Borrowing from composting, models of aerobic degradation of landfills can be divided, by means of their spatial distribution, into: (1) point, “lumped” or “batch” models, which consider the whole landfill as a “point” with constant properties, and (2) spatially distributed models that take into consideration the spatial variation of distributed parameters.

First order batch models were used by Haug (1993), Baptista et al. (2010), Mohee et al. (1998), Higgins and Walker (2001) and Mason (2008a). Monod or Contois type expressions for the solid waste biodegradation were used in works of Kaiser (1996), Lin et al. (2008), Qin et al. (2007) and Xi et al. (2008). Sole-Mauri et al. (2007) set up a more complex, integrated, two-stage biochemical model using Monod type kinetics for the hydrolysis process and a first-order kinetic growth of microorganisms. Finally, Petric and Selimbašić (2008) used a Runge–Kutta–Fehlberg method with approximation of fourth and fifth order and adjustment of step size for a n-order (n = 2.8944) lumped biodegradation model.

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However, due to the spatial variations of temperature, oxygen concentration, pH, free pore space, waste heterogeneity and other uncertainty, lumped models may fail to predict the mean behavior of the batch waste bioreactor. This can be more significant in landfills, where the air pressure gradient distribution across the different wells is not generally equal in space, resulting in variant mass and heat transfer in the landfill. Even for forced aeration composting, Bari and Koenig (2000, 2012) emphasized the need of spatially distributed models for pilot and field scale applications. Spatial and/or temporal distributed models in composting systems were used by Finger et al. (1976), VanderGheynst et al. (1997), Nakayama et al. (2007) and Bongochgetsakul and Ishida (2008). El-Fadel et al. (1996a, 1996b, 1997) developed and applied one of the first temporal and spatial distributed models for the generation and transport of gas in an (anaerobic) sanitary landfill.

The Waste Management Research Group of the University of Southampton (UK) developed the “Landfill Degradation And Transport” model (LDAT), which was recently released on-line in the Group’s web-site (http://www.wmrg.soton.ac.uk/). White et al. (2003, 2004), White and Nayagum (2011) and White and Beaver (2013) applied this to simulate biochemical degradation of solid waste in landfills for anaerobic conditions. Beaver et al. (2008), Rees-White et al. (2008a, 2008b) and Nayagum et al. (2009a) used it for aeration process simulation, calculating biochemical as well as flow field properties. The above mentioned sophisticated model includes an integrated biochemical model coupled with a flow simulation module that takes into consideration the degradation and settlement of the wastes and is well sustained by experimental investigations, for example the works of Rees-White et al. (2008a), Powrie and Beaver (1999) and Zardava et al. (2009).

Flow through waste solid matrix is usually considered as porous medium flow, generally simulated with Darcy’s formulation (Bear, 1972), accounting also for capillary suction and varying hydraulic conductivity as a function of liquid phase saturation. Fellner and Brunner (2010) studied the leachate generation from municipal solid waste landfills using the HYDRO-2D model and considering two different kinds of domains: a channel domain with high hydraulic conductivity and a matrix domain of slow water movement with high water retention capacity. Others simulated the groundwater and leachate flow after a landfill leachate leaking accident using in-house solver (Suto et al. 2006). Nayagum et al. (2009a, 2009b) simulated field-scale aerobic treatment applications, using forced-air injection, applying the LDAT model. Cestaro et al. (2003)
and Cossu and Cestaro (2005), applied the Darcy formulation in order to estimate the radius of influence of an aeration well.

Thus, although numerous works are available for the biodegradation process and the flow simulation modeling separately, there are only few models that combine them (e.g., LDAT). This is especially true for landfill aeration systems for which distributed models, combined with pilot scale applications, can be valuable for an optimum computer-aided design. Application of such a model could be useful to the aeration systems industry or to the research community, helping to understand and clarify the complex phenomena concerning aeration biochemical and hydrodynamic processes.

The objective of this work was to develop and primarily test a new model that will combine fluid mechanics and aerobic biodegradation modeling of landfilled organic solid waste. For this purpose, a multiphase flow model both for the air and liquid phase was used taking into consideration the oxygen transfer across gas and liquid phases. Liquid phase comprises the free pore water, which together with the moisture content of the waste constitute the total moisture of the system. Moreover, the capillary effect as well as the hydraulic conductivity as a function of moisture saturation was taken into consideration in the flow model. Oxygen enters the landfill in the unsaturated zone of waste matrix and is transferred in the gas and liquid phases under advection and dispersion mechanisms, as well as across phases under an interphase transfer mechanism, caused by oxygen concentration gradient. Furthermore, heat generation due to organics degradation or other biochemical processes was considered as source/sink term in the energy conservation equation. Finally, substrate and biomass participating in the biochemical reactions were simulated using chemical kinetics coupled with equations of the parameters that participate into reaction rates, such as oxygen transfer equations or energy equation for temperature calculation.

The novelty of the present work was the use of a multiphase computational approach that includes the capillary effect (unsaturated flow of water and air in the solid waste), combined with an interphase oxygen transfer and coupled with an organic matter biodegradation model. This model was developed using the commercial CFD solver ANSYS Fluent 14.0 (ANSYS, 2012) coupled with an extended in-house code that alters some parameters of the flow simulation program and simulates the biochemical process, in order to couple the mass/heat/species transfer equations with a biodegradation model for the organic solid waste. Simulation of landfill aeration is still a relatively new, unique and complex research area, with the first papers dating since 90s. The model in this paper could be used as a basis for aerations systems design and optimization, aiming at bringing landfill aeration modeling from research and development into the field of future practical design and applications.

2. Mathematical model development

In the present study, Computational Fluid Dynamics (CFD) techniques were applied for the multiphase simulation of landfill aeration process. Thus, the Control or Finite Volume (CV or FV) approach was used (LeVeque, 2002), which is included in the commercial solver ANSYS Fluent 14.0 algorithms. This was combined with an in-house developed code, using ANSI C programming language and “User Defined Functions” (UDFs) macro language of the ANSYS Fluent solver.

In order to simulate the rheological and biochemical characteristics of landfill aeration, a numerical code has to: (a) simulate the complex air–water flow in the unsaturated “porous” media of a landfill, (b) simulate oxygen species transfer in the gaseous (air) and aqueous (water) phase, taking into consideration the oxygen mass transfer between the different phases, (c) simulate the biochemical process of biodegradable solids fraction reduction and biomass production/decay system and (d) simulate effectively the heat production/consumption of the above biochemical processes.

Our in-house code:

- Defines the capillary effect in the momentum equations of the wetting phase (water).
- Defines the landfill hydraulic conductivity for the fluids of interest as a function of moisture saturation.
- Simulates the oxygen interfacial transfer between air–water interphase as well as the sink term due to biodegradation process.
- Simulates the heat source/sink term due to biochemical processes.
- Calculates the biodegradation factors, which participate in the kinetics of the biodegradation process, as well as the biodegradable solids and biomass concentration in the landfill.

2.1. Fluid flow equations

In the present study, each one of the phases taking part in the simulation was considered as a single continuum obeying a different set of momentum equations. Thus, the concept of Volume Fractions (VF) was used for each phase. VF represents the volume occupied by each phase. The laws of conservation of mass and momentum are satisfied by each phase individually, whereas the total continuity in a Control Volume (CV) is guaranteed using the conservation of VF mass law, expressed by an analytical equation for the sum of volume fractions of all phases that equals to one. This way, 100 per cent of free porous space is occupied by the sum of the aqueous or gaseous phase at all times.

The Navier–Stokes–Brinkman equations for an “Euler–Euler” multiphase approach (ANSYS, 2012) were used for the unsaturated flow, which is an extended Darcy’s model, for the simulation of momentum conservation in each CV. An expression of the above equations in a compact notation is:

\[
\frac{\partial (\phi \rho_a q_a)}{\partial t} + \nabla \cdot (\phi \rho_a q_a \mathbf{V}_a) = -\rho_a \nabla P + \nabla \cdot \sigma_{ae} + \rho_a \mathbf{g} - \frac{\mu_a}{\kappa} \nabla \cdot \mathbf{V}_a - \phi \rho_a \nabla P_a
\]

where \( \phi \) is the total porosity of the medium (dimensionless), \( q_a \) is the volume fraction of q phase (m³/m³), \( \rho_a \) is the density of q phase (kg/m³), \( \mathbf{V}_a \) is the Darcy velocity of the q phase, \( \sigma_{ae} \) is the dynamic viscosity of q phase, \( P \) is the static pressure (Pa), \( \mathbf{g} \) is the acceleration of gravity (m/sec²), \( \mu_a \) is the viscous stress (Pa), \( \kappa \) is the intrinsic or saturated permeability of q phase (m²), \( k_r \) is the relative permeability (dimensionless) calculated according to van Genuchten (1980) formulation. For the aquatic phase:

\[
k_r = S_r^{0.5} \left( 1 - S_r^{1/7} \right)^2
\]

For the gaseous phase:

\[
k_r = (1 - S_r)^{0.5} \left( 1 - S_r^{1/7} \right)^2
\]

where \( S_e \) is the saturation calculated as:

\[
S_e = \frac{a_{aw} - a_{ar}}{a_{aw} - a_{ar}}
\]

where \( a_{aw} \) is the volume fraction of the wetting phase (water), \( a_{ar} \) is the residual saturation, \( a_{aw} \) is the maximum (saturat) water content, and \( \gamma \) is the dimensionless van Genuchten constant.
The capillary pressure term \( \gamma_a \rho_g \nabla P_c \) is included only in the wetting phase, where \( P_c \) (Pa) is calculated using van Genuchten (1980)–Mualem (1976) formula:

\[
P_c = -\rho_g \frac{\gamma_a}{\alpha} \left( \frac{1}{\theta} \right)^{1/\beta}
\]

where \( \rho_g \) is the aqueous phase density (kg/m\(^3\)) and \( \alpha (1/m) \) and \( \beta \) are the van Genuchten constants \( (\gamma = 1 - \frac{1}{\beta}) \).

In Fig. 1, estimation of capillary pressure versus degree of saturation for the present work is compared and compared to various estimations of the capillary suction by previous works. Data by Wu et al. (2012) and Stoltz et al. (2012) were added to a previously published figure by Zardava et al. (2009). It is shown that present work values for the van Genuchten constants \( \alpha, \beta \) and \( \gamma \), taken from the University of Southampton (2008) LDAT project, result in a capillary pressure curve close to the “scatter” of the previous studies data. However, the values of \( \alpha, \beta \) and \( \gamma \) are different from those presented in the recent study by Wu et al. (2012). This can be explained due to the material properties heterogeneity that can cause different estimations of hydro-mechanical properties of solid wastes. This uncertainty can be overcome by conducting field or pilot tests in the examined area of interest.

A continuity equation is solved for each phase (ANSYS, 2012):

\[
\frac{\partial \rho_a q_a}{\partial t} + \nabla \cdot (\rho_a q_a V_a) = \dot{i} S_q
\]

where \( S_q \) is the mass source/sink term of the \( q \) phase.

In order to calculate the volume fraction of the examined phases, the equation for the sum of volume fractions of all phases, that equals one, is also used.

\[
\sum_{i=\text{gas, liquid}} a_i = 1
\]

2.2. Interface mass transfer and advection–dispersion–reaction equations

For oxygen mass transfer one advection–dispersion–reaction equation was solved for each phase, taking into consideration the interface mass transfer mechanism. The main reason for this mass transfer is the concentration gradient between the phases. The equilibrium concentration of oxygen in the liquid phase was calculated using Henry’s law expressed as:

\[
\text{C}_{\text{eq}, \text{O}_2} = \text{C}_{\text{O}_2}^\infty H_e(T)
\]

where \( \text{C}_{\text{eq}, \text{O}_2} \) is the equilibrium concentration of oxygen in the liquid phase, \( \text{C}_{\text{O}_2}^\infty \) is the equilibrium concentration of oxygen in the gas (gaseous) phase and \( H_e(T) \) is the dimensionless form of Henry's constant as a function of temperature \( T \), calculated form Sander (1999):

\[
H_{\text{II}}(T) = H_{\text{II}}^o \cdot \exp \left( -\frac{1}{T_0} \frac{1}{T} \right)
\]

where \( H_{\text{II}}^o \) is the dimensioned Henry’s constant (M/atm) at \( T_o \) (K) temperature, \( H_{\text{II}} \) is the constant of exponential decrease \( K \) and \( T \) is the temperature (K). The relation between dimensioned and dimensionless Henry’s constants is \( T \cdot H_{\text{II}}(T) = 12.2 H_{\text{II}}^o(T) \) (Sander, 1999). In Table 1 values of Henry’s constant (M/atm) for \( \text{O}_2 \) at 25 °C as well as the exponential decrease constant \( \alpha \) (1/K) values of various studies are presented.

The oxygen mass flow rate between the phases was calculated using the following expression (Weber and DiGiano, 1996):

\[
R_{\text{O}_2} = \rho_p \rho_a K_{\text{O}_2} \left( \text{C}_{\text{O}_2}^\infty - \text{C}_{\text{O}_2} \right)
\]

where \( R_{\text{O}_2} \) is the mass flux of oxygen from phase \( q \) to phase \( p \) with \( R_{\text{O}_2} = -K_{\text{O}_2} \) (kg/s m\(^3\)), \( \rho_a \) is the volume fraction of phase \( p \) (m\(^3\)/m\(^3\)), \( \rho_p \) is the density of \( p \) phase (kg/m\(^3\)), \( K_{\text{O}_2} \) is the mass transfer rate of oxygen from phase \( q \) to phase \( p \) (s\(^{-1}\)), \( \text{C}_{\text{O}_2}^\infty \) is the equilibrium concentration of oxygen in phase \( p \) (kg \( \text{O}_2 \)/kg \( \text{O}_2 \)), \( \text{C}_{\text{O}_2} \) is the concentration of \( C \) species in the phase \( p \) (kg \( \text{O}_2 \)/kg \( \text{O}_2 \)).

Thus, the oxygen mass transfer in each phase was simulated using the following advection–dispersion–reaction equation for each phase (ANSYS, 2012):

\[
\frac{\partial \rho_a q_a C_{\text{O}_2}^\infty}{\partial t} + \nabla \cdot (\rho_a q_a V_a C_{\text{O}_2}^\infty) = -\dot{i} q_a \rho_a C_{\text{O}_2}^\infty \nabla J + S_{\text{O}_2}
\]

Table 1 Values of Henry’s constant (M/atm) for \( \text{O}_2 \) at 25 °C and exponential decrease constant (K) of various studies.

<table>
<thead>
<tr>
<th>( \alpha ) (K)</th>
<th>( H_{\text{II}}^o ) at 25 °C</th>
<th>References</th>
</tr>
</thead>
<tbody>
<tr>
<td>1700</td>
<td>1.30 × 10(^{-3})</td>
<td>Sander, 1999</td>
</tr>
<tr>
<td>1800</td>
<td>1.20 × 10(^{-3})</td>
<td>Carpenter, 1966</td>
</tr>
<tr>
<td>1600</td>
<td>1.30 × 10(^{-3})</td>
<td>University of Southampton (2008)</td>
</tr>
<tr>
<td>1800</td>
<td>1.30 × 10(^{-3})</td>
<td>Present study</td>
</tr>
</tbody>
</table>

\(^*\) This value is equivalent to 4.24 × 10\(^{-1}\) kPa\(^{-1}\), which is the actually used value by the University of Southampton LDAT model. The LDAT model uses volumetric units to express concentration (m\(^3\)/m\(^3\)) and kPa for pressures.

Fig. 1. Capillary pressure vs. degree of saturation for municipal solid waste. (See above-mentioned references for further information.)
where \( \varepsilon \) is the total porosity of the medium (dimensionless), \( \phi_q \) is the volume fraction of \( q \) phase \((m^3/m^3)\), \( \rho_q \) is the density of \( q \) phase \((kg/m^3)\), \( C_{q0} \) is the oxygen concentration in \( q \) phase \((kg/m^3)\), \( V_q \) is the pore velocity of \( q \) phase \((m/s)\), \( S_O2 \) is the source/sink term of oxygen mass which includes the mass transfer of oxygen across the phases’ interface as well as the oxygen consumption due to the aerobic biodegradation of the substrate and \( J \) the dispersion term calculated using the Fick’s law:

\[
J = -D \times \nabla C_{q0}
\]

where \( D \) is the dispersion coefficient of oxygen \((m^2/s)\).

### 2.3. Energy conservation

Temperature is an important factor that affects the kinetics of the aerobic biodegradation. For the temperature field calculation, an energy conservation equation was solved for each phase (ANSYS, 2012):

\[
\frac{\partial \rho_q C_{p,q} T_q}{\partial t} + \nabla \cdot (\rho_q \phi_q V_q) = -\nabla \cdot \left( \rho_q C_{p,q} \mathbf{V}_q \right) + \rho_q C_{p,q} \chi_q + \rho_q c_{p,q} \right. + \nabla \cdot (\rho_q \phi_q \mathbf{V}_q - \nabla \phi_q) + S_q
\]

where \( \varepsilon \) is the total porosity of the medium (dimensionless), \( \phi_q \) is the volume fraction of \( q \) phase \((m^3/m^3)\), \( \rho_q \) is the density of \( q \) phase \((kg/m^3)\), \( h_q \) is the specific enthalpy of \( q \) phase \((J/kg \cdot K)\), \( v_q \) is the pore velocity of \( q \) phase \((m/s)\), \( P \) is the static pressure \((Pa)\), \( \tau \) is the shear stress \((Pa)\), \( S_p \) is the sink/source term of energy which includes the heat transfer across air–water as well as the energy production/consumption due to the biochemical processes taking place in the substrate (Section 2.4). The heat exchange between the different phases was calculated using the following equation:

\[
Q_{pq} = h_{pq}(T_p - T_q)
\]

where \( Q_{pq} \) is the heat transfer across the phases, having \( Q_{pq} = -Q_{qp} \), \( T_p \) is the temperature of \( p \) phase \((K)\), \( T_q \) is the temperature of \( q \) phase \((K)\) and \( h_{pq} \) is the volumetric heat transfer coefficient \((W/m^3 K)\) between the phases \( p \) and \( q \) calculated as a function of Nusselt number, using the Ranz and Marshal formulation (Ranz and Marshall, 1952a, 1952b).

### 2.4. Biodegradation equations and kinetics

The aerobic biodegradation of organic solid waste can be described by the following chemical mass balance equation (Tchobanoglous et al., 1993):

\[
(C_6H_7O_3)_d + \left(\frac{4a + b - 2c - 3d}{4}\right)O_2 \xrightarrow{\text{Biomass}} aCO_2 + \frac{(b - 3d)}{2}H_2O + dNH_3
\]

where \( a, b, c \) and \( d \) are constants referred to waste chemical composition. Numerous researchers have previously estimated and published values for these constants (e.g., Iannelli et al. (2005), Nikoli and Voudrias (2009) and Komilis et al. (2012)).

Reichel et al. (2005) and Sole-Mauri et al. (2007) proposed \( C_6H_7O_3N \) as a chemical formula for the biomass. The same chemical formula was used by others (Rees-White et al., 2008b; Nayagum et al., 2009b; University of Southampton, 2008) for bacteria growth equation:

\[
5C_6H_7O_3N_d + (a - 5d)NH_4^+ \xrightarrow{O_2} aC_3H_7NO_2 + (5b - 20d + a - 10c)H^+ + (5c - 2a)H_2O
\]

The corresponding chemical equation for the biomass decay, used by University of Southampton (2008), Rees-White et al. (2008b) and Nayagum et al. (2009b), was the following:

\[
C_6H_2NO_2 + 3H_2O + H^+ \xrightarrow{5/6C_3H_2O_6 + NH_4^+}
\]

The coupling of Eqs. (15) and (16) rate is usually achieved using the “yield coefficient” concept. Thus, kinetics of solid waste biodegradation and biomass production are connected with the following relationship:

\[
S_s = \frac{dC_s}{dt} = \frac{S_s}{V_q} = 1 \frac{dC_s}{dt}
\]

where \( S_s \) is the solid waste biodegradation rate \((kg/m^3 s)\), \( C_s \) is the concentration of the biodegradable solid waste \((kg/m^3)\), \( t \) is the time \((s)\), \( S_s \) is the biomass production rate \((kg/m^3 s)\), \( C_b \) is the biomass concentration in the waste matrix \((kg/m^3)\) and \( Y_b \) is the yield coefficient which connects kinetics of biodegradable solid waste and biomass \((kg_b/m^3 s/kg_s m^3 s)\).

In the present study two types of biochemical kinetics combined with corresponding correction factors were applied. The first type of kinetics was based on the Monod equation which in its generality is:

\[
S_s = \frac{dC_s}{dt} = \frac{k_m}{K_s + C_s} C_b
\]

where \( k_m \) is the maximum biodegradation rate in high biodegradable solids concentration \((s^{-1})\) and \( K_s \) is the half saturation constant for the solid waste \((kg/m^3)\).

Monod kinetics has been previously used by various researchers (Qin et al., 2007; Rees-White et al., 2008b; Lin et al., 2008; Xi et al., 2008; Nayagum et al., 2009a; Nayagum et al., 2009b) for aerobic biodegradation of solids.

The second type used first order kinetics, in order to evaluate the effect of kinetic choice on the results. First order kinetics was applied by the majority of previous works; suggestively the works of Higgins and Walker (2001), Mason (2008a), Baptista et al. (2010). The rate equation has the form:

\[
S_s = \frac{dC_s}{dt} = -k' C_s
\]

The most important parameters that affect aerobic biodegradation kinetics are (Haug, 1993 and Baptista et al., 2010): (1) the temperature, (2) the oxygen concentration, (3) the moisture content in waste, (4) the free air space that affects whether air can flow across the waste, (5) particle size that prescribes the effective surface of solid matrix where biodegradation occurs and (6) the pH.

In order to take into consideration the above mentioned parameters Haug (1993) proposed the following formula:

\[
S_s = \frac{dC_s}{dt} = -k' C_s = -k \times k_{temp} \times k_{mic} \times k_{O2} \times k_{pH} \times k_{FAS} \times k_{pH} \times C_s
\]

where \( k' \) is the effective/corrected biodegradation rate \((s^{-1})\), \( k \) is the maximum biodegradation rate \((s^{-1})\), \( k_{temp} \) is the temperature correction function (dimensionless), \( k_{mic} \) is the moisture content correction function (dimensionless), \( k_{O2} \) is the oxygen concentration correction function (dimensionless), \( k_{pH} \) is the free air space correction function (dimensionless) and \( k_{FAS} \) is the pH correction function (dimensionless).

In the present study correction factors only for temperature and oxygen were used. Free air space correction factor was not included in the applied kinetics, however this was taken into account in the present complex flow model, because volume fraction of air varies across the solid matrix affecting its distribution as well as oxygen transfer across the phases. Other correction factors, such as moisture content and pH were not considered in work. However, as water is considered as a moving fluid in the waste, oxygen and thus biodegradation kinetics is affected due to the free pore water.
For temperature, the following correction function was used, originally proposed by Rosso et al. (1993), which is based on the cardinal temperatures $T_{\text{min}}$, $T_{\text{max}}$ and $T_{\text{opt}}$:

$$k_{\text{temp}} = \frac{(T - T_{\text{opt}}) \times (T - T_{\text{min}})^2}{(T_{\text{opt}} - T_{\text{min}}) \times [(T - T_{\text{opt}}) \times (T - T_{\text{max}}) \times (T_{\text{opt}} + T_{\text{min}} - 2T)]}$$

(22)

where $T_{\text{min}}$ is the minimum acceptable temperature (${^\circ}$C or K), $T_{\text{max}}$ is the maximum acceptable temperature (${^\circ}$C or K) and $T_{\text{opt}}$ is the optimum temperature for the aerobic biodegradation (${^\circ}$C or K) and $T$ is the actual temperature (${^\circ}$C or K).

The above mentioned empirical formula has been applied by Sole-Mauri et al. (2007), Mason (2009), Baptista (2009) and Baptista et al. (2010). Although numerous correction functions acceptably fit experimental data in the literature, Mason (2006) concluded that Rosso’s empirical model, despite its empirical origin, includes a more easily estimated set of parameters which has a physical meaning in terms of composting/aerobic biodegradation.

The following correction function was used for the oxygen, where $C_{O_2}$ is the concentration of oxygen (kg/m$^3$) and $K_{O_2}$ is the half saturation constant for the oxygen (kg/m$^3$):

$$k_{O_2} = \frac{C_{O_2}}{K_{O_2} + C_{O_2}}$$

(23)

Using the above mentioned kinetics combined with Eq. (18), it is possible to calculate both the consumption of the biodegradable solid waste and the production of biomass. In addition to biomass production, biomass concentration is affected by bacterial decay rate $k_d$ (s$^{-1}$). For the biomass decay $S_D$ first order kinetics was assumed, which took into consideration the effect of temperature, using the correction $k_{temp}$, calculated by the empirical formula of Lin et al. (2008):

$$S_D = k_d K_{temp} C_B$$

(24)

with $k_{temp}$ calculated as:

$$k_{temp} = 2.147 \times 10^{-4} T^2 - 2.356 \times 10^{-2} T + 1.348 \quad (5 \; ^{\circ}C < T < 75 \; ^{\circ}C)$$

(25)

For the biomass production the values for $T_{\text{min}}$, $T_{\text{max}}$ and $T_{\text{opt}}$ were taken from Baptista et al. (2010). The quadratic function of Eq. (25) reaches its minimum value at 55 $^{\circ}$C (Lin et al., 2008) which is close to 58.6 $^{\circ}$C that corresponds to the optimum composting temperature in the work of Baptista et al. (2010).

Temperature of each phase was calculated from energy Eq. (13). Heat release due to biochemical reactions 15–17 was calculated using biochemical kinetics and formation enthalpy of each species. Values for the enthalpy of formation for the included species are shown in Table 2.

### 3. Numerical solution

#### 3.1 Parameter estimation

Table 3 presents the values of hydraulic parameters of solid wastes, used in the present study. As expected, all these values vary due to material heterogeneity and uncertainty and are highly site-dependent. Intrinsic permeability $k$ can be calculated as:

$$k = \frac{H}{\rho g}$$

(26)

where $k$ is the intrinsic permeability ($m^2$), $K$ is the saturated hydraulic conductivity ($m/s$), $\mu$ is the dynamic viscosity of the fluid (kg/m/s), $\rho$ is the density of the fluid (kg/m$^3$) and $g$ is the acceleration of gravity (m/s$^2$).

Hydraulic conductivity values of municipal solid waste depend on waste density, which is influenced by compaction and effective stress associated with depth of burial and varies by several orders of magnitude, e.g., 3.7 $\times$ 10$^{-8}$ to 1.5 $\times$ 10$^{-4}$ m/s (Powrie and Beaven, 1999) and 5.4 $\times$ 10$^{-8}$ to 6.1 $\times$ 10$^{-7}$ m/s (Jain et al., 2006). Landva et al. (1998) determined hydraulic conductivity in the order of 2 $\times$ 10$^{-8}$ to 2 $\times$ 10$^{-5}$ m/s in the vertical direction and 4 $\times$ 10$^{-4}$ to 1 $\times$ 10$^{-3}$ m/s in the horizontal direction defining a difference of 0(10$^3$) order between the horizontal and the vertical directions ($k_h/k_w \approx 0.10$), which is in the range 0.10 $< k_h/k_w < 0.25$ reported by Hudson et al. (2009) and the corresponding values from their literature review O(10$^{-2}$) $< k_h/k_w < O(10^0)$.

### Table 2

<table>
<thead>
<tr>
<th>$z$</th>
<th>Species</th>
<th>Symbol</th>
<th>Molecular weight</th>
<th>Enthalpy of formation</th>
<th>References</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Solid waste$^a$</td>
<td>$C_{6}H_{9}O_{3}.56N_{0.32}$</td>
<td>142.44</td>
<td>$-15073.4$</td>
<td>University of Southampton (2008)</td>
</tr>
<tr>
<td>2</td>
<td>Oxygen</td>
<td>$O_{2}$</td>
<td>32</td>
<td>$-365.94$</td>
<td>Benjamin (2002)</td>
</tr>
<tr>
<td>3</td>
<td>Carbon dioxide</td>
<td>$CO_{2}$</td>
<td>44</td>
<td>$-9528.64$</td>
<td>Wikipedia (2012)</td>
</tr>
<tr>
<td>4</td>
<td>Water</td>
<td>$H_{2}O$</td>
<td>18</td>
<td>$-18579.40$</td>
<td>Benjamin (2002)</td>
</tr>
<tr>
<td>5</td>
<td>Ammonia</td>
<td>$NH_{3}$</td>
<td>17</td>
<td>$-4722.94$</td>
<td>Benjamin (2002)</td>
</tr>
<tr>
<td>6</td>
<td>Ammonium ion</td>
<td>$NH_{4}^{+}$</td>
<td>18</td>
<td>$-7361.11$</td>
<td>Benjamin (2002)</td>
</tr>
<tr>
<td>7</td>
<td>Hydrogen ion</td>
<td>$H^{+}$</td>
<td>1</td>
<td>0.0</td>
<td>Benjamin (2002)</td>
</tr>
<tr>
<td>8</td>
<td>Biomass</td>
<td>$C_{6}H_{7}NO_{2}$</td>
<td>99</td>
<td>$-13790.9$</td>
<td>University of Southampton (2008)</td>
</tr>
<tr>
<td>9</td>
<td>Glucose</td>
<td>$C_{6}H_{12}O_{6}$</td>
<td>180</td>
<td>$-7061.11$</td>
<td>Wikipedia (2012)</td>
</tr>
</tbody>
</table>

$^a$ In kJ/kg.

$^b$ For Iannelli et al. (2005) chemical composition.
Default values of kinetic parameters used in the present study are listed in Table 4. These values have been chosen after an extensive literature review on aerobic biodegradation processes. Due to the lack of landfill experimental data, most of the included parameters were taken from other aerobic biochemical processes, such as composting. Kim et al. (2007) simulated both aerobic and anaerobic solid waste biodegradation in landfills, estimating maximum biodegradation rate to be 1 day\(^{-1}\) for the used Monod kinetics. Cardinal temperatures for the Rosso’s temperature correction factor have been widely used in the literature. Sole-Mauri et al. (2007) used a cardinal temperature correction factor for both mesophilic and thermophilic bacteria choosing \(T_{\text{min}} = 5.1\, ^\circ\text{C}\), \(T_{\text{opt}} = 35.4\, ^\circ\text{C}\) and \(T_{\text{max}} = 44.0\, ^\circ\text{C}\) for the former and \(T_{\text{min}} = 30.8\, ^\circ\text{C}\), \(T_{\text{opt}} = 57.2\, ^\circ\text{C}\) and \(T_{\text{max}} = 65.5\, ^\circ\text{C}\) for the latter. Mason (2008b) determined, after a sensitivity analysis, the values of \(T_{\text{min}} = 5.0\, ^\circ\text{C}\), \(T_{\text{opt}} = 59.0\, ^\circ\text{C}\) and \(T_{\text{max}} = 71.0\, ^\circ\text{C}\). Baptista et al. (2010) determined a slightly different set of values with \(T_{\text{min}} = 5.0\, ^\circ\text{C}\), \(T_{\text{opt}} = 58.6\, ^\circ\text{C}\) and \(T_{\text{max}} = 71.6\, ^\circ\text{C}\), which was adopted in the present model. The biodegradable solid waste half saturation constant value of 1 kg/m\(^3\) (Rees-White et al., 2008b) and oxygen half saturation constant value of 0.007 \times 10^{-3} \text{ kg/m}^3\) (Sole-Mauri et al., 2007) were used. Biomass decay rate value of 0.05 day\(^{-1}\) (Kim et al., 2007) and yield coefficient \(Y_s\) value of 0.1 (Beaven et al., 2008) were adopted. The same value for \(Y_s\) was applied by Rees-White et al. (2008b) and Nayagum et al. (2009a,b).

Finally, default material properties of liquid and gaseous phase included in the computational flow model are presented in Table 5.

These values have been taken from ANSYS Fluent database of fluid properties (ANSYS, 2012).

### 3.2 Model assumptions and solution methods

The following main assumptions were applied for model development:

- Aqueous and gaseous phase flow in the landfilled solid waste matrix was described as unsaturated porous media multiphase flow obeying the equations of Section 2.1.
- Solid waste matrix was assumed to be rigid (non-deformable).
- Flow was considered to be incompressible.
- Thermal equilibrium was assumed between solid waste and surrounding or contained fluids.
- Biodegradable solid waste as well as biomass were assumed to be in fixed positions.
- Biodegradation was assumed to take place in the liquid phase.

The commercial CFD solver ANSYS Fluent 14.0 was used, combined with an in-house developed code, using UDF macro language and ANSI C, in order to simulate the complex multiphase flow as well as the biochemical processes of landfilled solid waste aeration. More specifically, the “pressure-based” version of the solver was used. For the used partial differential equations, first-order spatial and temporal discretizations were used, while velocity–pressure coupling was achieved using “phase coupled SIMPLE” algorithm (ANSYS, 2012), which is a slightly modified multiphase version of the classic “SIMPLE” algorithm proposed by Patankar (1980). All biochemical equations were solved implicitly, while the flow model was coupled with the biochemical one using sink/source terms of the equations. Velocity magnitude in case of porous media flow is typically low and convergence criterion for all partial differential equations was set low, achieving convergence when all velocity components, mass and energy accuracy attain values of 10\(^{-12}\).

### 4. Results and discussion

In this section simulation results using the above described model are presented and analyzed. Due to the lack of extensive experimental data for landfill aeration, most of the comparisons
are either theoretical or come from similar aerobic processes (e.g., composting). In cases, where experimental results of previous studies were used, values of some of the needed parameters were not available and thus they were assumed to have typical values.

4.1. Comparison with experimental results

In the works of University of Southampton (2008), Rees-White et al. (2008b) and White and Heaven (2008) investigated solid waste aeration in typical bays 24 m long, 8 m wide and 3 m deep, where solid wastes were placed. Geometry of this application was considered as a two dimensional (2D) plane with 3 m depth and 8 m width. Air was assumed to enter the solid body through a 2 m wide inlet, which was located at the left bottom corner, while the top surface was completely open. Hydraulic properties of solid waste were assumed to be those of Table 3. Solid waste chemical formula was assumed to be that of Iannelli et al. (2005) (C₆H₆O₃₅N₀₃₂). Definition of proper boundary conditions is essential for the solution of the flow partial differential equations. In the present application three kinds of boundary conditions were used (Fig. S1):

- The “pressure inlet” boundary condition, which is mathematically described as a Dirichlet boundary condition for the relative pressure, was expressed as: \( P_{\text{inlet}} = P_0 \) where \( P_0 \) is the relative pressure (Pa) at the inlet. Similar boundary conditions were assumed both for the species mass transfer and temperature at inlet: \( C_{\text{inlet}} = C_0 \) and \( T_{\text{inlet}} = T_0 \). Where \( C_0 \) (kg/kg) and \( T_0 \) (K) represent the values of species concentration and temperature at the inlet.
- The “pressure outlet” boundary condition, which is a Dirichlet boundary condition for the relative pressure, was assumed to be \( P_{\text{outlet}} = P_0 \), where \( P_0 \) is the relative pressure (Pa) at the outlet. For the species mass transfer a zero flux boundary \( \frac{C_{\text{outlet}}}{C_0} = 0 \) condition was assumed, whilst for the temperature the following Dirichlet boundary condition was applied: \( T_{\text{outlet}} = T_0 \), where \( T_0 \) (K) was the temperature value at outlet.
- The “impermeable rigid wall” boundary condition, which is mathematically a Dirichlet boundary condition, for the velocity assuming no-slip condition \( V_W = 0 \text{ m/s} \), whereas for the species mass transfer and temperature a zero flux boundary condition was used: \( \frac{C_{\text{wall}}}{C_0} = 0 \) and \( \frac{T_{\text{wall}}}{T_0} = 0 \).

Fig. S1 presents the 2D examined geometry and the used boundary condition surfaces.

The model simulated a period of 1.5 days. During this period, pressure at the inlet was assumed to increase linearly from 40 Pa to 500 Pa over a period of 0.4 days (9.6 h), when it reached steady state. These pressure values, for the given hydraulic properties of the material, correspond to a flow rate of 0.2 m³/h m² at the end of the first hour, while the steady state air flow rate equals 1 m³/h m². Due to the fact that the analysis was conducted in 2 dimensions, the flow rates are expressed per area of the inlet. Relative pressure propagation during the linear increase of the pressure at the inlet and its distribution in Pa as well as velocity direction vectors of the gaseous phase, are shown in Fig. S2 for several time instants, when time equals 2, 4, 6, 8 and 16 h. This model capability of capturing transient flow simulations can be useful for aeration well simulation even using hybrid well simulation, which changes its operation both for gas introduction and extraction in the landfill.

Rees-White et al. (2008b) and Nayagum et al. (2009a) presented results of temperature measurements and simulation results of LDAT model in a 3 m deep stack. Initial conditions of the simulation, taken from Rees-White et al. (2008b) are: for the biodegradable solids \( C_S = 200 \text{ kg/m}^3 \), aerobic biomass concentration \( C_B = 1 \text{ kg/m}^3 \), pore water volume fraction \( a_W = 0.28 \text{ m}^3/\text{m}^3 \), oxygen concentration in air \( O_2 = 0.177 \text{ kg/m}^3 \) and temperature \( T_0 = 21.3 \text{ °C} \). Hydraulic characteristics were assumed to be the same with the previous application. The pressure at the inlet was set 3000 Pa which corresponds to a flow rate of 5.4 m³/h m². Simulations were carried out for two different biochemical kinetics, namely the Monod and first order kinetics, in order to evaluate the effect of kinetic choice. Results of the present model at \( z = -0.5 \text{ m} \) and \( z = -1.5 \text{ m} \) with the corresponding experimental measurements (for \( z = 1.0 \text{ m} \)) and LDAT results (for \( z = 0.5, 1.5 \) and 2.5 m) by Rees-White et al. (2008b) are shown in Fig. 2 (Analysis for different air flow rates can be seen in the “Supplementary data” section). Qualitative analysis of Monod and first order kinetics results both seem to be close to experimental results and LDAT results, for the chosen parameters. The Pearson coefficient for the Monod kinetics equals 0.9878 whilst the corresponding value for the first order kinetics is 0.9760 (both correlations are significant at the 0.001 level). Thus, Monod kinetics has a slightly stronger correlation to the experimental results.

Petric and Selimbašić (2008) developed and validated their mathematical lumped model for composting process simulation. In their experimental work, they used a laboratory 32-L cylinder reactor (0.48 m height × 0.30 m internal diameter), where 12.5 kg (experiment 2) of organic waste was placed. Organic waste mixture comprised 84% poultry manure on dry weight whilst the organic matter of the waste was 80.22% on dry weight. The initial total moisture was 69.11%, however due to the fact that the present model simulates the flow of the pore water, volume fraction of free water was assumed to be 32%. Air entered the reactor from the base with a flow rate of 0.18 m³/h. The organic matter conversion was calculated according to Eq. (27) (Petric and Selimbašić 2008):

\[
O_{MC} = \frac{\left[ \frac{OM_{\text{init}}}{100} \right] - \left[ \frac{OM_{\text{t}}}{100} \right]}{\frac{OM_{\text{init}}}{100} - \left[ \frac{OM_{\text{t}}}{100} \right]} 
\]

where \( OM_{\text{init}} \) is organic matter at the beginning of the process and \( OM_{\text{t}} \) is the instantaneous organic matter. The agreement between the results of organic matter conversion of the present model simulation and the experimental data by Petric and Selimbašić (2008) seems adequate (Fig. 3).

A model sensitivity analysis is presented in the “Supplementary Data” section of the paper.

![Fig. 2. Comparison of temperature results of the present model versus experimental measurements and LDAT model results of Rees-White et al. (2008b).](image-url)
4.2. Simulation of aeration wells

In this section, a preliminary analysis of aeration wells is described. First, computational analysis of a single aeration well was conducted in order to estimate its radius of influence. Then, these single well simulation preliminary results were used as a guide, in order to design and set the location of aeration wells in a hypothetical landfill aeration application, using multiple wells.

For the single aeration well simulation, a 2D field of 20.0 m × 20.0 m was considered, in the middle of which a well with Ø150 mm inner diameter was located. Permeability and the other hydraulic parameters were assumed to be those of Table 3, while solid waste biodegradation was assumed to follow Monod kinetics with its parameters defined in Table 4. A relative pressure difference of 5000 Pa was set in the inlet of the well and the geometry outer boundaries were considered open (pressure outlet boundary condition). This pressure difference is within the range of 20–80 mbars reported by Ritzkowski and Stegmann (2012) for low pressure aeration wells. The corresponding flow rate for this pressure difference is 2.2 m$^3$/h m. A period of 25 days was simulated.

**Fig. 3.** Organic matter conversion of the present study model versus experimental measurements by Petric and Selimbasic (2008).

**Fig. 4.** (a) Simulation of relative pressure distribution (Pa) for a single well. (b) Gaseous phase oxygen concentration in kg/m$^3$, as a function of radial distance from the well. Inlet pressure difference was assumed to be 5000 Pa and waste $k$ equals $10.23 \times 10^{-11}$ m$^2$. 
In Fig. 4a, the pressure distribution (in Pa) of the simulated single well is shown between inlet pressure value and that of 2 cmH2O (196 Pa). The latter was the relative pressure limit used by Cossu and Cestaro (2005) to define the radius of influence in their field work. The radius of influence resulting from such a pressure distribution is 7.5 m. In another case study, Cossu and Cestaro (2005) determined a radius of influence 10–14 m, based on oxygen concentration ("oxygen radius"). Using our model simulations, we computed an oxygen radius of 11.2 m using a threshold of 13.5% v/v O2 (~0.18 kg/m³) (Fig. 4b).

Using 7.5 m radius of influence for a single well, we proceeded to an aeration system design. Thus, a theoretical field of 45 m x 45 m was considered where 9 wells are installed. In Fig. 5, the examined geometry is presented. Some of the installed wells are used for air introduction (positive pressure wells) and some are vacuum wells (negative pressure wells). At blowing wells, pressure was assumed to be 5000 Pa, whilst at the corresponding negative pressure wells, pressure was −5000 Pa. These values correspond to air flow rates of 15 m³/h m and 18 m³/h m. In order to evaluate the effect of sucking/blowing schedule on solid waste biodegradation, two different schedules were simulated. In the first one, sucking/blowing wells are considered as those of Fig. 5, while in the second one, wells alter their behavior during the simulation following a square wave pattern between 5000 Pa and −5000 Pa pressure (hybrid wells), changing their operation every two days.

Typical results of relative pressure distribution and velocity direction vectors between the positive and negative pressure wells are shown in Fig. 6. Radial flow is typical, representing a flow direction from the positive pressure wells to the negative ones.

Moreover, solid waste biodegradation at two monitoring points A and B (see Fig. 5) are plotted in Fig. 7, both for the constant and
Due to the lack of extensive integrated experimental data, comparison of the results of the present work was conducted using literature experimental data from a single point in space (Rees-White et al., 2008b and Petric and Selimbašić, 2008). Temperature results of the present model (using both Monod and first order kinetics) seem to be in adequate agreement with the corresponding experimental results and University of Southampton LDAT model of Rees-White et al. (2008b). Furthermore, comparison was carried out using measured biodegradation rate results from Petric and Selimbašić (2008). Agreement between measurements of the latter work and present model was considered again sufficient. However, additional verification and validation of the present work using integrated experimental results in two and three dimensions is essential.

Simulation results of aeration wells showed that both pressure and concentration calculated fields can be useful for aeration systems design. The radius of influence of an aeration well was estimated by defining a “limit” value for relative pressure at radial distance from the well. Results of the single well were used in order to locate more wells in a theoretical landfill field. Single well simulations are useful for the landfill aeration systems design; however interaction between wells has to be taken into consideration during design process. Finally, comparing results of constant behavior wells with those of hybrid blowing/sucking wells, it was shown that the latter was more efficient in terms of solid waste biodegradation, due to the entrance of fresh cool air in the region.

5. Conclusions

In the present work, a new time and space integrated model for the numerical simulation of landfill aeration, using computational fluid dynamics techniques, was developed and presented. The present model development was based on the use of the commercial CFD solver ANSYS Fluent and an in-house code that alters the main solver and simulates the biochemical processes of landfill aeration. Taking into consideration the unsaturated hydraulics of solid waste and the complex biochemical processes, the present model calculates both the flow and biochemical field in the solid waste matrix.

Due to the lack of extensive integrated experimental data, comparison of the results of the present work was conducted using...
Management and Landfill Symposium, S. Margherita di Pula, Cagliari, Italy, 5–9 October.


