

A FEM simulation of transport and conversion processes in landfills using a multiphase model based on the theory of porous media

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Zusammenfassung

Weltweit betrachtet ist die Deponierung von Abfällen die verbreitetste Art, Abfälle zu entsorgen. Das damit verbundene Gefährdungspotenzial für die Umwelt bleibt auch nach der Ablagerungsphase bei einer zeitlich sukzessiv sinkenden Intensität der ablaufenden Deponieprozesse über Jahrzehnte erhalten. Insbesondere das durch Mikroorganismen aus den organischen Abfallanteilen gebildete Deponiegas mit seinen beiden Hauptbestandteilen Methan (CH_4) und Kohlendioxid (CO_2) führt bei unkontrollierten Emissionen neben einem explosiven Gefährdungspotenzial (CH_4) zu einer Beschleunigung des anthropogen bedingten Klimawandels. Darüber hinaus kann das bei der Deponierung entstehende Sickerwasser zur Kontamination des anstehenden Bodens und des Grundwassers führen. Eine Abschätzung des Langzeitverhaltens einer Deponie in Bezug auf die Sickerwassermengen, den Abbau der organischen Substanz, die daraus resultierende Gasproduktion und den damit verbundenen Setzungen ist für Planer, Deponiebetreiber und Abfallbehörden u.a. zur Dimensionierung und Genehmigung von Anlagenteilen, sowie zur Einschätzung der Dauer der Nachsorgephase und des Gefährdungspotenzials unerlässlich. Als Hilfsmittel werden dafür häufig Prognosemodelle verwendet. Viele der existierenden Modelle sind jedoch nicht in der Lage, die stark miteinander gekoppelten Prozesse innerhalb einer Deponie adäquat zu beschreiben, sowie zeitlich und räumlich abzubilden.

Aus dieser Motivation heraus wurde ein Deponiemodell basierend auf der Theorie poröser Medien für Mehrphasensysteme entwickelt. Dabei werden die gekoppelten Transport- und Umsetzungsprozesse innerhalb einer Deponie durch mathematisch gekoppelte Differentialgleichungen beschrieben, die mit Hilfe der Finiten Elemente Methode (FEM) numerisch gelöst werden. Das entwickelte Deponiemodell erlaubt damit eine zeitliche und räumliche (3-D) Darstellung der gekoppelten Deponieprozesse in Bezug auf die Entwicklung des vorhandenen Organikgehalts, der Abbaurate, der Temperatur, der Dichte des Abfallgemisches, der Setzungen und der Gasentwicklung. Hierbei werden die Einflüsse der Deponiegeometrie und -geometrie berücksichtigt. Die lokale Berechnung der Gasbildungsrate, des Gasdruckes und der daraus resultierenden Gasströmung zu jedem Zeitschritt ermöglicht eine Simulation der diffus über die Deponieoberfläche austretenden Gasemissionen. Bei der zusätzlichen Berücksichtigung eines mit Unterdruck betriebenen Gaserfassungssystems ist mit Hilfe des Simulationsmodells eine Optimierung des aktiven Gaserfassungssystems durch die Identifizierung von über- und untersaugten Deponiebereichen möglich.

Die vorliegende Arbeit zeigt den theoretischen Hintergrund des entwickelten Deponiemodells mit den aufgestellten Feldgleichungen (Konzept der Volumenanteile, Sättigungsbedingung, Massen-, Impuls-, Drall- und Energiebilanz), den zur Schließung des Gleichungssystems erforderlichen konstitutiven Materialgleichungen (einschließlich der Auswertung der Entropieungleichung für einen thermodynamisch konsistenten Modellsatz), sowie die numerische Aufbereitung der Gleichungen zur Implementierung in das 'Finite Element Analysis Program' FEAP. Durch die Identifizierung und Bestimmung der erforderlichen physikalischen und chemischen Materialparameter der einzelnen Konstituierenden kann ein realistisches Materialverhalten des Abfallgemisches unter Deponiebedingungen simuliert werden, wobei sich der Einfluss einzelner Materialparameter auf das Simulationsergebnis anhand der durchgeführten Sensitivitätsanalyse erkennen lässt. Die Validierung des Modells erfolgte u.a. durch die Simulation der Deponieprozesse einer in den 80er und 90er Jahren errichteten bzw. betriebenen Siedlungsabfalldeponie und dem anschließenden Vergleich der Simulationsergebnisse mit vorhandenen Messdaten.

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Abbreviations and symbols

Greek letters

α	Identifier of the 1, ..., κ individual constituents (phases) φ^α
α^m	Thermal expansion coefficient of the mixture or individual materials
$\alpha^{\alpha R}$	Real thermal expansion coefficient of the constituent φ^α
$\alpha_{\nabla\Theta}$	Heat conductivity of the mixture
$\alpha_{\nabla\Theta}^{\alpha R}$	Real heat conductivity of the constituent φ^α
$\beta, \beta_1, \beta_2, \beta_i$	Fitting parameters for temperature and pH-function
$\beta_p, \beta_m, \beta_t$	Fitting parameters of applied temperature function (5.66) concerning psychrophilic, mesophilic and thermophilic microorganisms
$\partial(\dots)$	Partial derivative concerning the quantity (...)
$\partial^2(\dots)$	2. partial derivative concerning the quantity (...)
$\Delta(\dots)$	Change in the quantity (...)
ε^α	Specific internal energy of the constituent φ^α
η^α	Specific entropy of the constituent φ^α
$\eta_{CH_4}, \eta_{CO_2}, \eta_{LG}$	Dynamic viscosity of methane, carbon dioxide and landfill gas
Θ	Temperature
Θ^α	Temperature of the constituent φ^α
Θ_{0S}	Temperature at reference configuration
$\Theta_{opt,p}, \Theta_{opt,m}, \Theta_{opt,t}$	Optimum temperature of metabolism activity concerning psychrophilic, mesophilic and thermophilic microorganisms
$\Theta_{225}, \Theta_{465}$	Local temperature at point 225 and point 465
κ	Number of individual constituents
$\kappa_p, \kappa_m, \kappa_t$	Fitting parameters of applied temperature function (5.66) concerning psychrophilic, mesophilic and thermophilic microorganisms
$\lambda, \lambda^{OR}, \lambda^{GR}$	Lagrange multiplier
$\lambda, \lambda_{LG}, \lambda_W$	Heat conductivity of individual materials, landfill gas and water
μ	Specific growth rate of microorganism(s)
μ_{max}	Maximum specific growth rate of microorganism(s)
μ_1, μ_2, μ_J	Chemical potential concerning the substance 1, 2 and J

ν, ν_j	Stoichiometric coefficients, concerning the substance J
ρ	Total density of the mixture
ρ^α	Partial density of the constituent φ^α
$\rho^{\alpha R}$	Real density of the constituent φ^α
$\hat{\rho}^\alpha$	Mass supply term of the constituent φ^α
$\hat{\rho}^O$	Organic degradation rate
$\hat{\rho}_{225}^O, \hat{\rho}_{465}^O$	Local organic degradation rate at point 225 and point 465
$\hat{\rho}_{\max}^O$	Maximum organic degradation rate
$\hat{\rho}_\Theta^O$	Dimensionsless function of temperature influencing $\hat{\rho}^O$
$\hat{\rho}_n^O$	Dimensionsless function of organic content influencing $\hat{\rho}^O$
$\hat{\rho}_{\text{pH}}^O$	Dimensionsless function of pH-value influencing $\hat{\rho}^O$
$\hat{\rho}_w^O$	Dimensionsless function of water content influencing $\hat{\rho}^O$
$\hat{\rho}_i^O$	Dimensionsless function of further inhibitors influencing $\hat{\rho}^O$
$\hat{\rho}_{\text{energy}}$	Amount of exchanged energy
$\sum$	Sigma sign (summation operator)
ψ^α	Helmholtz free energy of the constituent φ^α
Ψ^α	Chemical Potential of the constituent φ^α
Ψ_{tot}	Total porosity
φ^α	Individual constituent α
χ	Motion function
χ_α	Lagrangean motion function of the constituent φ^α
χ_α^{-1}	Eulerian Motion function of the constituent φ^α
∂B_S	Boundary area of the solid phase (material surface area)

Latin letters

$(\dots)^{-1}$	Inverse of the quantity (...)
$(\dots)^T$	Transpose of the quantity (...)
$(\dots)_{0S}^0$	The quantity (...) of the constituent φ^α in the reference configuration (initial condition)
$[\dots]^T$	Equilibrium concentration of the quantity [...]
$[A], [B], [C], [D], [J]$	Concentration of the chemical substance A, B, C, D and J
$[E], [ES]$	Concentration of enzymes and enzyme-substrate complex
$[P], [S]$	Concentration of product and substrate
a, b, c, d	Corresponding stoichiometric coefficients of substances A, B, C, D
A	Pre-exponential factor in ARRHENIUS equation
$\mathbf{A}_\alpha$	Almansi strain tensor in the actual configuration
AbfAblV	Abfallablagerungsverordnung
ATP	Adenosine triphosphate
b	Regression coefficient in the RATKOWSKY equation
b_j	Molality of the substance J in solution
$\mathbf{b}$	Acceleration due to gravity
B	Control space of an investigated body
B_{0S}	Control space of an investigated porous solid body in the reference configuration ($t_0 = 0$)
B_S	Control space of an investigated porous solid body in the actual configuration ($t_1 > t_0$)
B_S^+	Control space of an investigated porous solid body in the actual configuration ($t_2 > t_1$)
$\mathbf{B}_\alpha$	Left Cauchy Green deformation tensor
BMU	Bundesministerium für Umwelt, Naturschutz und Reaktorsicherheit
BOD ₅	Sum parameter: biological oxygen demand after 5 days
°C	Degree of Celsius
$\mathcal{C}$	Set of constitutive quantities
$c^{\alpha R}$	Real specific heat capacity of the constituent φ^α
c_j	Molar concentration of the substance J in solution
C_{Inh}	Concentration of an inhibitor
C_J	Concentration of the substance J

C_{Oxy}	Concentration of oxygen
C_P, C_S	Product concentration and substrate concentration
C_{Pm}	Maximum product concentration where specific growth rate is zero
C_X	Concentration of microorganisms
$\mathbf{C}_\alpha$	Right cauchy green deformation tensor
CAD	Computer-aided design
COD	Sum parameter: Chemical oxygen demand
$\mathcal{D}$	Set of the dissipative part
$d(\dots)$	Derivative of the quantity (...)
da, da	Surface element in the actual configuration
$d\mathbf{A}_{0\alpha}$	Surface element in the reference configuration
$\mathbf{D}_\alpha$	Symmetric part of the spatial velocity gradient $\mathbf{L}_\alpha$
DepV, DepVerwV	Deponieverordnung, Deponieverwertungsverordnung
$\det(\dots)$	Determinant of the quantity (...)
DFG	Deutsche Forschungsgesellschaft (German Research Foundation)
$\text{div}(\dots)$	Divergence of the quantity (...) concerning actual configuration
DK I, DK II	Deponieklasse I (landfill class I), Deponieklasse II (landfill class II)
dm	Dry matter
DNA	Deoxyribonucleic acid
dv	Bulk volume element
dv^α	Volume element of the constituent φ^α
dv^G	Volume element of the gas phase, representing the void volume which is permeable for the gas phase
$dV_{0\alpha}$	Volume element in the reference configuration
$d\mathbf{x}$	Differential line element in the actual configuration
$d\mathbf{X}_\alpha$	Differential line element in the reference configuration
$e^{(\dots)}, e^{(\dots)}$	Exponential function
$\hat{e}^\alpha$	Internal energy supply term of the constituent φ^α
E	Enzymes
E	Internal Energy
E_A	Activation energy in ARRHENIUS equation
E_m	Molar internal Energy

E^α	Internal energy of the constituent φ^α
$\mathbf{E}_\alpha$	Green strain tensor
ES	Enzyme-substrate complex
$\mathcal{F}$	Set of field quantities
$f(\dots)$	Function of the quantity $(\dots)$
$\mathbf{F}_\alpha$	Deformation gradient of the constituent φ^α
$\mathbf{F}_\alpha^+$	Adjoint tensor of $\mathbf{F}_\alpha$
FE, FEM	Finite Element, Finite Element Method
G	Gas
G	Gibbs energy
G_{col}	Collectable specific gas potential
G_e	Specific gas potential
G_m	Molar Gibbs energy
G_t	Cumulated specific gas production at the time t
$\bar{G}_J$	Partial molar Gibbs energy of the substance J
GAMBIT	CAD programme
$\text{grad}(\dots)$	Gradient of the quantity $(\dots)$ concerning actual configuration
$\text{Grad}(\dots)$	Gradient of the quantity $(\dots)$ concerning reference configuration
h_{tot}	Total height
$\mathbf{h}_{(0)}^\alpha$	moment of momentum of the constituent φ^α referred to the spatial point 0
H	Entropy
H_m	Molar entropy
H^α	Entropy of the constituent φ^α
$\bar{H}_J$	Partial molar entropy of the substance J
HDPE	High density polyethylene
I	Inert
$\mathbf{I}$	Identity tensor
J	Joule
J_α	Jacobian
$\mathcal{K}$	Set of known field quantities
k	Empirical constant in a AIBA kinetic of microbial growth
k	Rate constant
k_1	Rate constant of the forward reaction

k_2	Rate constant of the forward reaction in a multi step reaction
k_{-1}	Rate constant of the backward reaction
k_{cat}	Rate constant of a catalytic reaction
$\mathbf{k}^\alpha$	Resulting force vector on the constituent φ^α
K	Fourth constant in a EDWARDS kinetic of microbial growth
K	Equilibrium constant
K	Kelvin
K	Kinetic energy
K^α	Kinetic energy of the constituent φ^α
K_0	Intrinsic permeability
K_I	Dissociation constant
K_I	Inhibition constant
K_M	MICHAELIS-MENTEN constant
K_{no}	Organic saturation constant within the developed landfill model
K_{Pi}	Product inhibition constant
K_S	Substrate saturation constant
kg	Kilogram
kg_{dm}	Kilogram referred to dry matter
kg_{Org}	Kilogram referred to biodegradable organic matter
kg_{wm}	Kilogram referred to wet matter
l	Liter
$\mathbf{I}^\alpha$	Momentum of the constituent φ^α
$\hat{\mathbf{I}}^\alpha$	Supply term of momentum of the constituent φ^α
$\ln(\dots)$	Natural logarithm
L	Liquid
$\mathbf{L}_\alpha$	Spatial velocity gradient
LDPE	Low density polyethylene
LG	Landfill gas
LOI	Loss of ignition
m	Mesophilic
m	Mass
m_{solvent}	Mass of the solvent
m^α	Mass of the constituent φ^α
$\hat{m}^\alpha$	Mass supply term of the constituent φ^α

m, m^2, m^3	Meter, square meter and cubic meter
$\mathbf{m}_{(0)}^\alpha$	Sum of all external moments
$\hat{\mathbf{m}}_{(0)}^\alpha$	Sum of internal moments
M	Molar mass
MB	Methanogenic biomass
MBT	Mechanical-biological waste (pre-)treatment
ME	Metals
MI	Minerals
MSW	Municipal solid waste
month	Month
$(\dots)^n$	Level of exponent
$n, n_1, n_2, n_i, n_J, n_k$	Amount of substances, amount of substance 1, 2, i, J and k
n^α	Volume fraction of the constituent φ^α
n_{0S}^α	Initial volume fraction of the constituent φ^α
n^G	Volume fraction of the gas phase (permeable porosity)
n_{225}^O, n_{465}^O	Volume fraction of organic at point 225 and point 465
$\mathbf{n}$	Unit normal vector
N, N_0	Final cell number, initial cell number
Nm^3	Standard cubic meter
NO	Native organics
O	Organic
$\mathcal{P}$	Set of independent process variables
p	Pressure
p	Psychrophilic
$\hat{\mathbf{p}}^\alpha$	Local interaction force of the constituent φ^α
P	Precipitation
P	Product
PA	Polyamide
PE	Polyethylene
pH	pH-value
PP	Polypropylene
PS	Polystyrene
PU	Polyurethane
PVC	Polyvinyl chloride
$\mathbf{q}$	Heat flux vector

$\mathbf{q}^\alpha$	Heat flux vector of the constituent φ^α
Q, Q_P, Q_V	Heat, rate of heat under constant pressure, constant volume
Q^α	Rate of heat of the constituent φ^α
$\mathcal{R}$	Set of free available quantities
$r, r_{\max}$	Rate of reaction, maximum rate of reaction
r_b, r_f	Rate of backward reaction, rate of forward reaction
r^α	Internal heat source of the constituent φ^α
R, R^G	General gas constant
R_S^G	Specific gas constant
RL	Richtlinie
RNA, rRNA	Ribonucleic acid, ribosomal ribonucleic acid
RVE	Representative volume element
s	Second
S	Inorganic solid phase
S	Substrate
S	Enthalpy
S_m	Molar enthalpy
$\bar{S}_J$	Partial molar enthalpy of the substance J
SD	Standard deviation
SI, SI-unit	International system of units
SM	Synthetic matter
t	Time
$t_{1/2}$	Half life
$\mathbf{t}^\alpha$	Local surface force
T	Temperature
$T_{\min}, T_{\max}, T_{\text{opt}}$	Minimum, maximum and optimum temperature
$\mathbf{T}^\alpha$	Cauchy stress tensor of the constituent φ^α
TAA	Technische Anleitung zur Lagerung, chemisch/physikalischen, biologischen Behandlung, Verbrennung und Ablagerung von besonders überwachungsbedürftigen Abfällen
TASI	Technische Anleitung zur Verwertung, Behandlung und sonstigen Entsorgung von Siedlungsabfällen
TM	Theory of mixture
TOC	Total organic carbon
TPM	Theory of porous media

$\mathbf{u}$	Displacement vector
$\mathcal{V}_{(...)}$	Number of (...)
v, v	velocity, velocity of a reaction
V	Volume
V_{m}	Molar volume
V^{α}	Partial volume of the constituent φ^{α}
$\bar{V}_{\text{H}_2\text{O}}$	Partial molar volume of water
$\bar{V}_{\text{J}}$	Partial molar volume of the substance J
VFA	Volatile fatty acid
vs	Versus
$\mathbf{w}_{\text{GS}}$	Difference velocity between the gas phase and the solid phase
$\mathbf{w}_{\text{OS}}$	Difference velocity between the organic phase and the solid phase
W	Water
W	Watt
W	Work, rate of work
W^{α}	Rate of work of the constituent φ^{α}
$\mathbf{W}_{\alpha}$	Skew symmetric part of the spatial velocity gradient $\mathbf{L}_{\alpha}$
wm	Wet matter
x_{j}	Mole fraction
$\mathbf{x}$	Position vector in the actual configuration
$\mathbf{x}'_{\alpha}$	Velocity of the constituent φ^{α}
$\mathbf{x}''_{\alpha}$	Acceleration of the constituent φ^{α}
X	Extensive state variable
X_{α}	Material point of the constituent φ^{α}
$\mathbf{X}_{\alpha}$	Position vector of the constituent φ^{α} in the reference configuration
$\bar{X}, \bar{X}_{\text{J}}$	Partial molar quantity, partial molar quantity of the substance J
Y	Yield coefficient
$z[\text{m}]$	Height (given in meter)

Chemical Compounds

C, C(s)	Carbon, in a solid state of aggregation (graphite)
C ₄ , C ₅ , C ₆ , C ₇ , C _n	Number of carbon atoms contained in a chemical compound
C _{Org}	Biodegradable organic carbon
Ca	Calcium
CH ₄ , CH ₄ (g)	Methane, in a gaseous state of aggregation
CH ₃ COO ⁻ (aq)	Acetate in a aqueous state of aggregation
C _n H _a O _b	Unspecific organic compound
C ₅ H ₈ O ₄	Hemicellulose
C ₆ H ₁₀ O ₅	Cellulose
C ₆ H ₁₂ O ₆	Glucose
C ₁₂ H ₂₂ O ₁₁ (s)	Saccharose in a solid state of aggregation
CO ₂ , CO ₂ (g)	Carbon dioxide, in a gaseous state of aggregation
H ₂ (g)	Hydrogen in a gaseous state of aggregation
H ₂ O(g)	Water in a gaseous state of aggregation
H ₂ O(l)	Water in a liquid state of aggregation
HS ⁻	Inorganic sulfur compound
K	Potassium
Mg	Magnesium
N	Nitrogen
N ₂	Molecular nitrogen
Na	Sodium
NH ₃	Ammonia
NH ₄ -N	Ammonium
NO ₂ -N	Nitrite
NO ₃ -N, NO ₃ ⁻	Nitrate
O ₂ (g)	Oxygen in a gaseous state of aggregation
P	Phosphorus
S	Sulfur
SO ₄ ²⁻	Inorganic sulfur compound