BIODEGRADATION IN POROUS LANDFILL BODIES

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Summary In this contribution a constitutive model based on the macromechanical Theory of Porous Media (TPM) for a saturated thermo elastic porous body has been developed. The body under investigation consists of an organic and inorganic moisturized phases and a gas phase. Based on a consistent thermomechanical treatment the governing equations and constitutive equations will be given. Thus, we obtain a mathematical concept describing the motion of the solid phase, the pressure of the gas phase, the temperature of the mixture and the biodegradation of organic material into a gas mixture of methane and carbon dioxide produced by bacterial decomposition during stable methane fermentation (biogas).

INTRODUCTION

The Earth's average surface temperature rose by around 0.6 °C during the 20th century. It seems to be evidence that most of the global warming is caused by emissions of carbon dioxide (CO_2), methane (CH_4) and other greenhouse effect gases. Landfilling belongs to an important global sources of greenhouse gases. In this case, the time scale belongs to hundreds of years. Therefore, development of a numerical model describing the effect of solid phase composition (consisting of organic and inorganic materials) and the pore structure of the landfill body on the conversion phenomena and multi-component gas transport is of great importance. This has been done based on the well established Theory of Porous Media for which basic relations will be summarized in the following section.

MODELING

The Theory of Porous Media is the mixture theory restricted by the concept of volume fractions. Hereby, we consider a continuum which consists of several constituents. As aforementioned, the investigated porous body consists of φ^{S} (solid), φ^{O} (organic) and φ^{G} (gas). A porous medium occupying the control space of the porous solid $\mathrm{B_S}$, with the boundary $\partial\mathrm{B_S}$, consists of constituents φ^α ($\alpha = \mathrm{S,O,G}$) with real volumes v^α. The boundary $\partial\mathrm{B_S}$ is a material surface for the solid phase and a non-material surface for the liquid and gas phases. The volume fractions $\mathrm{n}^\alpha(\mathbf{x},\mathrm{t}) = \mathrm{dv}^\alpha/\mathrm{dv}$ refer the volume elements dv^α of each individual constituents φ^α to the bulk volume element dv. The main statement of the volume fraction concept can be founded by the saturation condition $\sum_\alpha^{\mathrm{SOG}} \mathrm{n}^\alpha(\mathbf{x},\mathrm{t}) = \sum_\alpha^{\mathrm{SOG}} \rho^\alpha/\rho^{\alpha\mathrm{R}} = 1$, see [1], wherein $\mathbf{x}$ is the position vector of the spatial point x in the actual placement and t is the time. Moreover, the partial density of the constituent φ^α, namely ρ^α, is related to the real density of the materials $\rho^{\alpha\mathrm{R}}$ involved via the volume fractions n^α. The concept of volume fractions is an important part of the theory following in the next sections. Due to the volume fraction concept, all geometric and physical quantities, such as motion, deformation and stress, are defined in the total control space. Thus, they can be interpreted as the statistical average values of the real quantities.

Field equations

The local statements of the balance equations of mass and of of momentum are given for the constituents φ^α by

$$(\rho^\alpha)'_\alpha + \rho^\alpha \operatorname{div} \mathbf{x}'_\alpha = \hat\rho^\alpha, \qquad \operatorname{div} \mathbf{T}^\alpha + \rho^\alpha(\mathbf{b} - \mathbf{x}''_\alpha) + \hat{\mathbf{p}}^\alpha - \hat\rho^\alpha\, \mathbf{x}'_\alpha = \mathbf{0}\,. \tag{1}$$

In (1), "div" denotes the divergence operator, $\hat\rho^\alpha$ represents the mass supply between the phases which has to conform to $\hat\rho^{\mathrm{S}} + \hat\rho^{\mathrm{O}} + \hat\rho^{\mathrm{G}} = 0\,,$ $\mathbf{T}^\alpha$ is the partial CAUCHY stress tensor, $\rho^\alpha\,\mathbf{b}$ specifies the volume force and $\hat{\mathbf{p}}^\alpha$ describes the interactions of the constituents φ^α which are restricted to $\hat{\mathbf{p}}^{\mathrm{S}} + \hat{\mathbf{p}}^{\mathrm{O}} + \hat{\mathbf{p}}^{\mathrm{G}} = \mathbf{0}$. Additionally, the balance of energy concerning the whole mixture body must be taken into account:

$$\sum_\alpha^{\mathrm{S,O,G}} \Big(\rho^\alpha \underbrace{[(\psi^\alpha)'_\alpha + (\theta^\alpha)'_\alpha\, \eta^\alpha + \theta^\alpha\, (\eta^\alpha)'_\alpha]}_{(\varepsilon^\alpha)'_\alpha} - \mathbf{T}^\alpha \cdot \mathbf{D}_\alpha - \rho^\alpha\, \mathrm{r}^\alpha \Big) =$$

$$= \sum_\alpha^{\mathrm{S,O,G}} \Big(-\operatorname{div} \mathbf{q}^\alpha + \hat{\mathrm{e}}^\alpha - \hat{\mathbf{p}}^\alpha\, \mathbf{x}'_\alpha - \hat\rho^\alpha (\underbrace{\psi^\alpha + \theta^\alpha\, \eta^\alpha}_{\varepsilon^\alpha} - \frac{1}{2}\, \mathbf{x}'_\alpha \cdot \mathbf{x}'_\alpha)\Big). \tag{2}$$

Herein, $(\psi^\alpha)'_\alpha$ and $(\varepsilon^\alpha)'_\alpha$ represent the material time derivation of the free HELMHOLTZ energy ψ^α and of the internal energy ε^α, respectively, θ^α is the temperature, η^α specifies the specific entropy, $\mathbf{D}_\alpha$ is the symmetric part of the spacial velocity gradient, r^α denotes the local external heat supply and $\mathbf{q}^\alpha$ is the heat influx vector. The local energy supply term $\hat{\mathrm{e}}^\alpha$ must satisfy the constrain condition $\hat{\mathrm{e}}^{\mathrm{S}} + \hat{\mathrm{e}}^{\mathrm{O}} + \hat{\mathrm{e}}^{\mathrm{G}} = 0$. At least, in order to close the set of equation, the saturation condition has to be taken into consideration.

Assumptions

The system is investigated under the condition of a compressible gas phase but an incompressible solid and organic phase and we imbibe that the immobile phases have the same motion: $(\rho^{\mathrm{SR}})'_{\mathrm{S}} = 0$, $(\rho^{\mathrm{OR}})'_{\mathrm{S}} = 0$, $\mathbf{x}'_{\mathrm{S}} = \mathbf{x}'_{\mathrm{O}}$. The liquid is assumed to be an integral part of organic and solid phase. Moreover, we assume the solid to be not involved in the mass transition: $\hat{\rho}^{\mathrm{S}} = 0$. In addition, the organic phase is neglected in respect to the interaction forces: $\hat{\mathbf{p}}^{\mathrm{O}} = \mathbf{0}$. In order to keep the numerical complexity in a manageable scope, we have made restrictions for all phases of small deformations, excluding accelerations and a unique temperature of all phases at the same place: $\mathbf{x}''_\alpha = \mathbf{0}$, $\theta^{\mathrm{S}} = \theta^{\mathrm{O}} = \theta^{\mathrm{G}} = \theta$.

Constitutive equations

From the evaluation of the entropy inequality of the the liquid and/or gas saturated porous body considering saturation condition as a constraint, see [1], we obtain the constitutive relations for $\mathbf{T}^\beta$ ($\beta = \mathrm{S}, \mathrm{O}$) and the mobile phase $\mathbf{T}^{\mathrm{G}}$:

$$\mathbf{T}^\beta = -\,\mathrm{n}^\beta\,\mathrm{p}^{\mathrm{GR}}\,\mathbf{I} + 2\,\rho^\beta\,\mathbf{F}_{\mathrm{S}}\frac{\partial\psi^\beta}{\partial\mathbf{C}_{\mathrm{S}}}\,\mathbf{F}_{\mathrm{S}}^{\mathrm{T}}, \qquad \mathbf{T}^{\mathrm{G}} = -\,\mathrm{n}^{\mathrm{G}}\,\mathrm{p}^{\mathrm{GR}}\,\mathbf{I}\,, \tag{3}$$

with the realistic gas pressure p^{GR}, the tensor of identity $\mathbf{I}$, the deformation gradient $\mathbf{F}_{\mathrm{S}}$ and the right Cauchy-Green tensors $\mathbf{C}_{\mathrm{S}}$ according to the solid. For the compressible gas phase, p^{GR} is related to the real density ρ^{GR} with the nonlinear expression: $\mathrm{p}^{\mathrm{GR}} = \mathrm{c}^{\mathrm{G}}_{\mathrm{p}}\ln(\rho_0^{\mathrm{GR}}/\rho^{\mathrm{GR}})$ wherein $\mathrm{c}^{\mathrm{G}}_{\mathrm{p}} = \rho_0^{\mathrm{GR}}\,\theta\,\mathrm{R}_{\mathrm{G}}$ denotes a parameter concerning the reference density ρ_0^{GR} and the specific gas constant R_{G}. From the evolution of the entropy inequality, see [2], we gain restrictions concerning the interaction force $\hat{\mathbf{p}}^{\mathrm{G}}$ and the heat flux $\mathbf{q}^{\mathrm{SOG}}$ with $\mathbf{q}^{\mathrm{SOG}} = \sum_\alpha^{\mathrm{S,O,G}}\mathbf{q}^\alpha$:

$$\hat{\mathbf{p}}^{\mathrm{G}} = \mathrm{p}^{\mathrm{GR}}\,\mathrm{grad}\,\mathrm{n}^{\mathrm{G}} + \theta\,\alpha^{\mathrm{G}}_{\mathbf{w}_{\mathrm{GS}}}\,\mathrm{grad}\,\theta - \theta\,\mathrm{S}_{\mathrm{G}}\,\mathbf{w}_{\mathrm{GS}}, \qquad \mathbf{q}^{\mathrm{SOG}} = -\,\alpha_\theta\,(\theta)^2\,\mathrm{grad}\,\theta - \alpha^{\mathrm{G}}_{\mathbf{w}_{\mathrm{GS}}}\,(\theta)^2\,\mathbf{w}_{\mathrm{GS}}. \tag{4}$$

Herein, “grad” denotes the gradient operator, $\alpha^{\mathrm{G}}_{\mathbf{w}_{\mathrm{GS}}}$ represents a value concerning the dependency between the heat flux and interaction forces and α_θ is the heat conductivity. Moisture content is an important influencing factor concerning heat conductivity. Moreover, S_{G} describes the interaction between the gas phase and the remaining constituents in connection with the seepage velocity $\mathbf{w}_{\mathrm{GS}}$ with $\mathbf{w}_{\mathrm{GS}} = \mathbf{x}'_{\mathrm{G}} - \mathbf{x}'_{\mathrm{S}}$. The material parameter function S_{G} is postulated in dependence of the volume fraction n^{L}, see [3]. The Ansätze concerning to the free Helmholz energy functions ψ^α have been taken over by [2]. However, an intensive investigation on ψ^α has to be exerted. The mass supply reads

$$\hat{\rho}^{\mathrm{O}} = -\,\delta^{\mathrm{O}}_{\psi^{\mathrm{OG}}}\,\frac{1}{\theta}(\Psi^{\mathrm{O}} - \Psi^{\mathrm{G}}) = -\,\delta^{\mathrm{O}}_{\psi^{\mathrm{OG}}}\,\mathrm{K}_{\mathrm{B}}\,(\frac{\theta-\theta_{0\mathrm{S}}}{\theta_{0\mathrm{S}}})\,\rho^{\mathrm{O}}, \tag{5}$$

wherein $\delta^{\mathrm{O}}_{\psi^{\mathrm{OG}}}$ defines a positiv constant for the chemical potential functions Ψ^{O} and Ψ^{G} , see [2], K_{B} denotes a parameter associated with active biomass and $\theta_{0\mathrm{S}}$ is the reference temperature. The organic mass supply expresses the changes in organic phase due to bacterial activity, by which degradable organic matter is degraded. The more organic waste presents in a landfill, the more landfill gas is produced by the bacteria during decomposition. Organic mass supply depends on substrate concentration, expressed as density of organic matter, active biomass and temperature.

Numerical Treatment

Within the framework of a standard GALERKIN procedure, weak formulations are formed. Under consideration of the assumptions as well as the constitutive equations we receive the set $\Re$ of unknown quantities $\Re = \Re(\mathbf{x},\mathrm{t}) = \{\mathbf{u}_{\mathrm{S}}, \mathbf{w}_{\mathrm{GS}}, \mathrm{n}^{\mathrm{S}}, \mathrm{n}^{\mathrm{O}}, \mathrm{n}^{\mathrm{G}}, \mathrm{p}^{\mathrm{GR}}, \theta\}$ wherein $\mathbf{u}_{\mathrm{S}}$ denotes the displacement of the solid phase. In order to develop an effective calculation concept, we insert the saturation condition, the integral statement of the balance of mass concerning the solid phase: $\mathrm{n}^{\mathrm{S}} = \mathrm{n}^{\mathrm{S}}_{0\mathrm{S}}\ \det\mathbf{F}_{\mathrm{S}}^{-1} = \mathrm{n}^{\mathrm{S}}_{0\mathrm{S}}\ \mathrm{J}_{\mathrm{S}}^{-1}$, into the set of equations. Therein $\mathrm{n}^{\mathrm{S}}_{0\mathrm{S}}$ denotes the reference volume fraction of the solid phase. Moreover, the seepage velocity concerning the gas phases $\mathbf{w}_{\mathrm{GS}}$ will be calculated using the balance of momentum in the DARCY formulation, see [3]. Finally, the set of unknown quantities $\Re$ can be reduced to $\Re = \Re(\mathbf{x},\mathrm{t}) = \{\mathbf{u}_{\mathrm{S}}, \mathrm{n}^{\mathrm{O}}, \mathrm{p}^{\mathrm{GR}}, \theta\}$.

CONCLUSION

A closed calculation concept for the simulation of thermal mass transition in porous media has been developed. An essential contribution is given by implementation of the thermal mass transfer on the basis of an thermodynamical and physical motivated investigation. To this subject, there have been many empirical approaches published but only a limited number of continuum mechanical treatments are known. The presented contribution in the framework of a “smeared” continua has led to reasonable field equations, and in particular, to proper constitutive equations for the stresses, interaction volume forces, heat flux and mass supply. Nevertheless, further investigations are necessary to fit the presented calculation concept in respect of landfill bodies.

References

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