Cemracs'15 Project: SiViBiR++
Simulation of a Virtual Bioreactor using Feel ++

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May 11, 2015

1 Introduction

The principle of the bioreactor landfill consists in accelerating the degradation of wastes stored in a waste disposal by bringing them an optimal humidity in particular by the recirculation of leachates. Bacteria decompose the waste producing several by-products including methane gas and leachate fluid. In order to control gas and leachate production in the bioreactor, we develop a multiphase flow model of a bioreactor landfill.

2 Mathematical model of the bioreactor

2.1 Geometrical domain

As shown in Figure 1, the geometrical domain of a bioreactor landfill is a 3-dimensional domain, relatively simple. Generally speaking it is not a parallelepiped but it is not that much complicated.
Within this domain their are drains (when they are horizontal) and wells (when they are vertical). Some of them are used to extract the gas. The others allows the recirculation of leachates. In figure 1, a well is represented.

The system of coordinates we use for position is x, y, z and t stands for the time.

2.2 Mathematical model

Carbon is consumed by the bacteria existing in the bioreactor, we then write the following equation:

$$\frac{\partial C^{\text{org}}}{\partial t}(x,y,z,t) = \\ -\alpha d_b(x,y,z,t) C^{\text{org}}(x,y,z,t)\,\Psi(\rho(x,y,z,t))\ \max\Big(1-\frac{|T(x,y,z,t)-T_{\text{opt}}|}{A_T},0\Big)\,, \quad (1)$$

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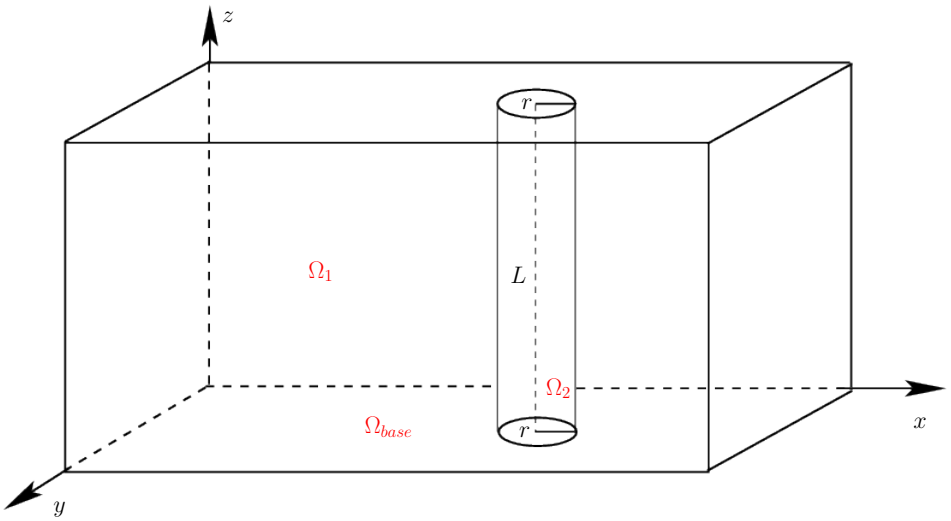

Figure 1: bioreactor landfill

where $C^{\text{org}}(x, y, z, t)$ is the spatial density of organic carbon, $d_b(x, y, z, t)$ is the spatial density of bacteria, $\rho(x, y, z, t)$ is the density of liquid water (the mass of liquid water by unit volume),

$$\Psi(\rho) = \rho \max\Big(1 - \frac{\rho}{\rho_{\text{Max}}}, 0\Big), \tag{2}$$

with ρ_{Max} being the density of liquid water at which the bioreactor is almost drowned, $T(x, y, z, t)$ is the temperature in (x, y, z) at time t, T_{opt} is the optimal temperature for the bacteria, A_T is the amplitude of temperature tolerated by the bacteria and α is a constant.
In this equation, expression

$$C^{\text{org}}(x, y, z, t)\, \Psi(\rho(x, y, z, t))\ \max\Big(1 - \frac{|T(x, y, z, t) - T_{\text{opt}}|}{A_T}, 0\Big), \tag{3}$$

is related to the metabolism of each bacterium. The last factor in this expression translates the fact that the metabolism is maximum when the temperature equals T_{opt} and that it is 0 when the temperature is further from T_{opt} by A_T. The two first factors say that this metabolism is in proportion to the quantity of carbon and to $\Psi(\rho)$. This quantity is proportional to liquid water around the bacterium when it is small and it is limited by ρ_{Max}; this means that the metabolism of bacteria is stopped in region of the bioreactor that are drowned.
Once this expression is multiplied by the spatial density of bacteria $d_b(x, y, z, t)$, one obtains something that is a measurement of the density of bacteria activity. Hence equation (1) says that the rate of organic carbon consumption is in proportion to bacteria activity, α being the proportion coefficient.

Consumption of organic carbon by bacteria produces methane, carbon dioxyde and water. we then write the following equation for methane density:

$$\frac{\partial M}{\partial t}(x, y, z, t) + u(x, y, z, t) \cdot \nabla M(x, y, z, t) = -c_M \frac{\partial C^{\text{org}}}{\partial t}(x, y, z, t), \tag{4}$$

where $u(x, y, z, t)$ is the velocity of gas in the bioreactor and where c_M is a proportionality constant.

We also write the following equation for carbon dioxyde density, $c_{C^{\rm dx}}$ being a proportionality constant:

$$\frac{\partial C^{\rm dx}}{\partial t}(x,y,z,t) + u \cdot \nabla C^{\rm dx}(x,y,z,t) = -c_{C^{\rm dx}} \frac{\partial C^{\rm org}}{\partial t}(x,y,z,t). \tag{5}$$

Water can exist in the bioreactor in two phases: liquid and vapor. This leads to write the two following equations for $\rho(x,y,z,t)$ and density of water vapor $h(x,y,z,t)$ (the mass of water vapor per unity volume):

$$\begin{aligned}\frac{\partial h}{\partial t}(x,y,z,t) + u(x,y,z,t) \cdot \nabla h(x,y,z,t) - c_h \Delta h(x,y,z,t) = \\ c \max\Big[H(T) - h(x,y,z,t), 0\Big]\rho(x,y,z,t) - \tilde{c} \max\Big[h(x,y,z,t) - H(T), 0\Big] \\ - c_{\rm wat} \frac{\partial C^{\rm org}}{\partial t}(x,y,z,t),\end{aligned} \tag{6}$$

$$\frac{\partial \rho}{\partial t}(x,y,z,t) + u_\rho \frac{\partial \rho}{\partial z}(x,y,z,t) - c_\rho \Delta \rho(x,y,z,t) = \tilde{c} \max\Big[h(x,y,z,t) - H(T), 0\Big] + \rho^{\rm add}, \tag{7}$$

with:

$$H(T) = H_0 - H_1 T, \tag{8}$$

where H_0 and H_1 are constants.

$H(T)$ in (8) stands for a threshold of density of water vapor underneath which liquid water turns to vapor. This threshold depends on the temperature : the larger the temperature the smaller this threshold.

In Equation (6), the evolution of water vapor is written according to the Fick's second law. The last term in (6) translates the fact that consumption of organic carbon produces waters.
The first term in the right hand side of (6) means that the production of vapor from liquid water is 0 as soon as the density of vapor is larger than threshold $H(T)$ (the air is saturated). If vapor density h is smaller than threshold $H(T)$, then the production of vapor is in proportion to available liquid water and to the gap between the vapor density and the threshold.
The second term in the right hand side of (6) means that the production of liquid water from vapor is 0 if the density of vapor is smaller than threshold $H(T)$. When vapor density h is larger than threshold $H(T)$, then the production of liquid water is in proportion to the gap between the vapor density and the threshold. This production of liquid water is removed from the vapor compartment.

It is also added, as a source term in equation (7). This equation is an advection-diffusion equation describing the evolution of liquid water. It contains a term (the second one in the left hand side) that translates the fact that liquid water flows down.
It also contains the term $\rho^{\rm add}$ which models the fact that leachates are added in the bioreactor This term is known.

Those two equations involve several constants: c_h, c, $\tilde{c}$, $c_{\rm wat}$, u_ρ and c_ρ.

The evolution of the temperature in the bioreactor is given by the heat equation with a source term due to the activity of bacteria, which is proportional to

$$\frac{\partial C^{\rm org}}{\partial t}(x,y,z,t), \tag{9}$$

thanks to (1). So the equation for the temperature reads:

$$\frac{\partial T}{\partial t}(x,y,z,t) - c_T \Delta T(x,y,z,t) = -\beta \frac{\partial C^{\rm org}}{\partial t}(x,y,z,t), \quad T\big|_{\partial\Omega} = T_{\rm ext}, \tag{10}$$

for two constants c_T and β.

The evolution of bacteria is also proportional to the activity of bacteria, we then write the following equation, for a constant c_d:

$$\frac{\partial d_b}{\partial t}(x,y,z,t) = -c_d \frac{\partial C^{\text{org}}}{\partial t}(x,y,z,t)). \tag{11}$$

The following equation describes the flow of leachate at the output of the bioreactor:

$$\frac{\partial L}{\partial t}(x,y,z,t) = \int_{\partial\Omega_{base}} \frac{\partial \rho}{\partial z}(x,y,z,t). \tag{12}$$

The gas inside the bioreactor also contains oxygen and nitrogen which density are solution to

$$\frac{\partial O}{\partial t}(x,y,z,t) + u(x,y,z,t)\cdot\nabla O(x,y,z,t) = 0, \tag{13}$$

$$\frac{\partial N}{\partial t}(x,y,z,t) + u(x,y,z,t)\cdot\nabla N(x,y,z,t) = 0. \tag{14}$$

The velocity u of gas in the bioreactor can be written as the gradient of a potential ϕ by the next equation:

$$u(x,y,z,t) = \nabla\phi(x,y,z,t), \quad (x,y,z)\in\Omega. \tag{15}$$

We assume that the gas is incompressible, the continuity equation for the gas can be written as:

$$\text{div}\left((M + C^{\text{dx}} + h + O + N)u\right)(x,y,z,t) = G^{\text{pump}}, \quad (x,y,z)\in\Omega. \tag{16}$$

Right hand side G^{pump}, which is known, models the fact that the gas is extracted from the bioreactor by pumping.
We then have according to (15) the Laplace equation:

$$\text{div}\left((M + C^{\text{dx}} + h + O + N)\nabla\phi\right)(x,y,z,t) = G^{\text{pump}}, \quad (x,y,z)\in\Omega, \tag{17}$$

to which we add the boundary condition :

$$\frac{\partial\phi}{\partial n}(x,y,z,t) = 0, \quad \text{on} \ \ \partial\Omega, \tag{18}$$

since the gas can glide along the boundary of the bioreactor.

3 Goal of the Cemracs project

The goal is to implement this model within Feel++. The constants, ρ^{add} and G^{pump} need to be parameters of the code to be developed as the initial data associated to every field of the model.

The coding needs to account for the fact that in the next steps

- the values of the constants will be adjusted using data,
- the initial data will be adjusted using data,
- the code will be used for the control of real bioreactors.