

SiViBiR++ project: Simulation of a Virtual Bioreactor Landfill using Feel++

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2 Modeling a bioreactor landfill

3 Implementation

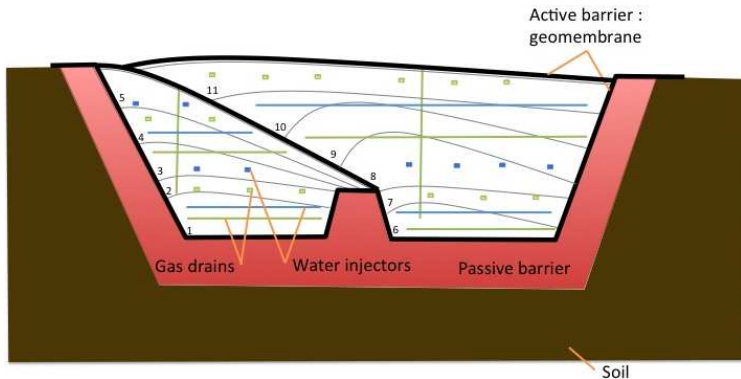
4 Numerical results

5 Conclusions

What is a bioreactor landfill?

A bioreactor landfill is a waste management facility that features:

- Decomposition of **organic wastes** (waste treatment)
- Production of **methane** and **heat** through the process (energy generation)

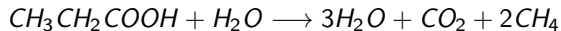


Dimension : $100m \times 50m \times 50m$, life expectancy : ~ 50 years
1 ton of waste can generate $100m^3$ of methane

A bioreactor landfill model

Functioning of a bioreactor landfill:

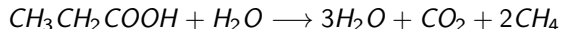
- Bacteria consume organic wastes (fats, carbohydrates, ...)



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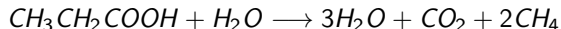


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- The reaction takes place in presence of *good* **temperature** and **humidity** conditions

A bioreactor landfill model

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Inputs and outputs:

- Methane is extracted by the drains (productors system)
- Liquid water is injected into the bioreactor to increase humidity and decrease the temperature (injectors system)

Goals of the SiViBiR++ project

SiViBiR++ project aims at answering the following questions:

- What are the **equations** describing the bioreactor landfill?
- How to **numerically** simulate a bioreactor landfill?
- Can we **predict** the quantity of gas that will be produced by the bioreactor landfill in the next 20/30 years?

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Meeting the players

The variables involved in the bioreactor landfill model are:

- Concentration of bacteria

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- Concentration of bacteria
- Concentration of organic carbon
- Concentration of liquid water
- Concentration of gas (methane, carbon dioxide, water vapor, oxygen and nitrogen)
- Temperature
- Velocity of the gas mixture

Bacteria production and organic carbon consumption

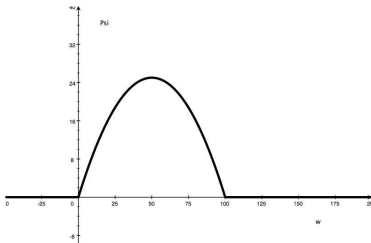
d_b : Concentration of bacteria

C^{org} : Concentration of organic carbon

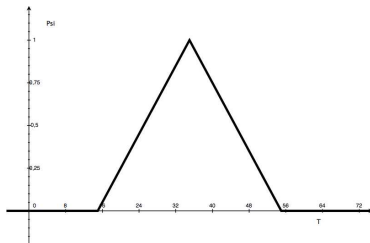
$$\begin{cases} \frac{\partial C^{\text{org}}}{\partial t} = -a d_b C^{\text{org}} \Psi(w) \tilde{\Psi}(T) \\ \frac{\partial d_b}{\partial t} = -c_d \frac{\partial C^{\text{org}}}{\partial t} \end{cases}$$

$\Psi(w)$ accounts for the *good conditions* of humidity

$\tilde{\Psi}(T)$ accounts for the *good conditions* of temperature



$\Psi(w)$, w : liquid water



$\tilde{\Psi}(T)$, T : temperature

Heat equation

The temperature T is solution of the classical heat equation

$$\frac{\partial T}{\partial t} - k_T \Delta T = -c_T \frac{\partial C^{\text{org}}}{\partial t}$$

The source term depends on the consumption of organic carbon during the reaction driven by the bacteria

Boundary conditions impose a given temperature on the external wall of the bioreactor and on the top membrane:

$$\begin{aligned} T &= T_{\text{ground}} && \text{on } \partial\Omega_{\text{wall}} \\ T &= T_{\text{membrane}} && \text{on } \partial\Omega_{\text{top}} \end{aligned}$$

Evolution of the gases and the water

Modeling the gases:

G : Concentration of a gas in the bioreactor

u : Velocity field

ϕ : Porosity of the wastes

$$\phi \frac{\partial G}{\partial t} + \underbrace{u \cdot \nabla G}_{\text{transport}} = \underbrace{f(t, x)}_{\text{source term}}$$

The source term is

- zero for oxygen (O) and nitrogen (N) $\Rightarrow f = 0$
- due to the consumption of C^{org} for methane (M) and carbon dioxide (C^{dx})
 $\Rightarrow f \propto -\frac{\partial C^{\text{org}}}{\partial t}$
- related to the condensation phenomenon for the water vapor (h)

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Modeling the water:

- Advection-diffusion equation with a vertical drift due to the gravity
- The source term reproduces the condensation phenomenon and the injection of liquid water

Velocity field

Hypothesis:

- Incompressible flow
- Darcy's law

$$\begin{cases} \nabla \cdot u = 0 \\ u = -\nabla \Phi \end{cases} \Rightarrow -\Delta \Phi = 0$$

Boundary conditions :

$$\begin{cases} u \cdot n = 0 & \text{on } \partial\Omega \\ u \cdot n = u_{\text{out}} & \text{on the drains} \end{cases}$$

Remark

The boundary condition on the drains may be rewritten as a source term concentrated on a line in the equation for the velocity field: $-\Delta \Phi = G^{\text{pump}}$

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Finite Element Embedded Library and Language in C++

A **Domain Specific Language** for PDE's embedded in C++ providing a syntax very close to the mathematical language

Features

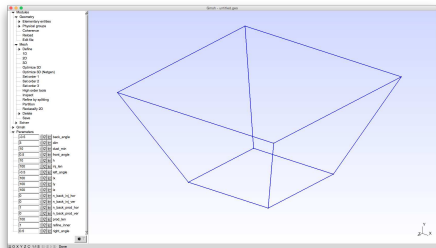
- Supports an arbitrary approximation order for Galerkin methods (cG, dG) in 1D, 2D and 3D
- Supports simplex, hypercube and high order meshes
- Supports seamless parallel computing
- Supports large scale parallel linear and non-linear solvers (PETSc/SLEPc)
- Supports mesh preprocessing (GMSH)

The geometry of the bioreactor landfill 1/2

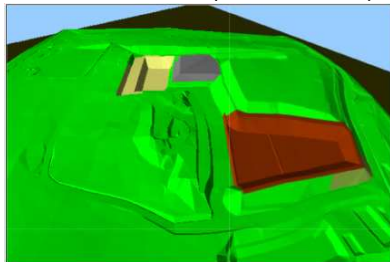
We focus on the alveolus 7b represented as a customizable box (the Chinese food box) to handle different geometries:

- Parametrized lengths, slopes, ...
- Varying slopes (shear transformations)

GMSH geometry



3D representation (Drouès landfill)



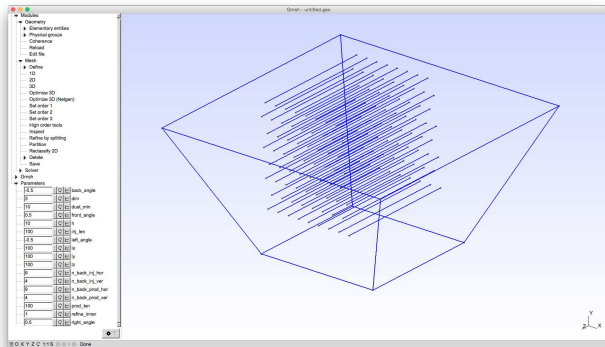
(Courtesy of Entreprise Charier)

The geometry of the bioreactor landfill 2/2

Two grids of small pipes model

- Water injectors
- Gas extraction system (producers)

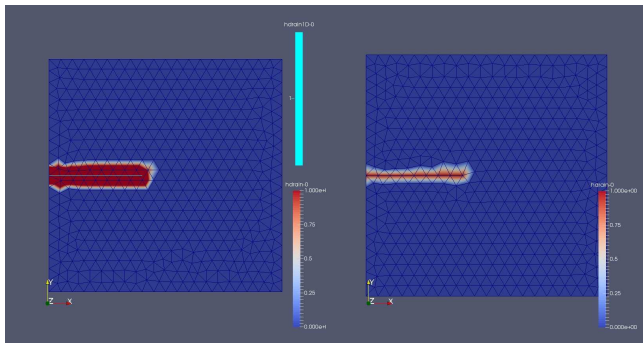
represented as 1D lines located inside the 2D/3D domain.



3D-1D coupling

Two methods to handle 1D lines in 3D geometries:

- 1D lines embedded in the 2D/3D mesh
⇒ Add constraints to the mesh (mesh size, partitions in parallel, ...)!
- Interpolation between 1D lines and 2D/3D meshes
⇒ High computational cost (Construction of the interpolation operator)

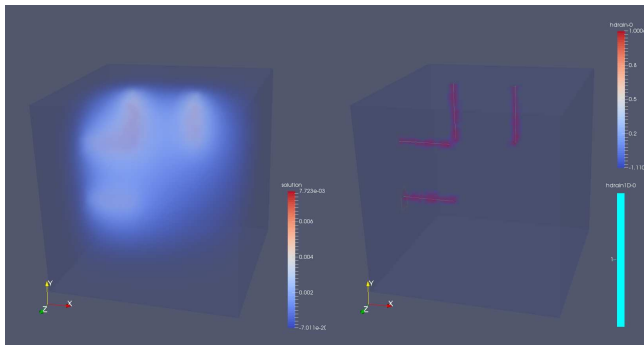


Interpolated line (left), Embedded line (right)

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Solution of the Laplace equation in 3D using Dirac masses over lines as source term

Approximation of the organic carbon and the temperature

- Semi-implicit treatment of the non-linear reaction term
- Explicit treatment of the coupling terms

At each time step, we seek C^{org} in the space of \mathbb{P}_1 Finite Elements such that

$$\int_{\Omega} \frac{C^{\text{org},n+1} - C^{\text{org},n}}{\Delta t} \Phi dx = - \int_{\Omega} a C^{\text{org},n+1} (d_b^0 + c_d C^{\text{org},0}) \Psi(w^n) \tilde{\Psi}(T^n) \Phi dx \\ + \int_{\Omega} a c_d C^{\text{org},n} C^{\text{org},n+1} \Psi(w^n) \tilde{\Psi}(T^n) \Phi dx$$

At each time step, we seek T in the space of \mathbb{P}_1 Finite Elements such that

$$\int_{\Omega} \frac{T^{n+1} - T^n}{\Delta t} \Phi dx + k_T \int_{\Omega} \nabla T^{n+1} \cdot \nabla \Phi dx = -c_T \int_{\Omega} \frac{\partial C^{\text{org},n}}{\partial t} \Phi dx$$

Approximation of the velocity field

We consider a **mixed formulation** for the velocity equation:

$$\begin{cases} \nabla \cdot u = G^{\text{pump}} \\ u = -\nabla \Phi \end{cases}, \quad u \cdot n = 0 \text{ on } \partial\Omega$$

We seek $(u, \Phi) \in H(\text{div}) \times L^2(\Omega)$ such that $u \cdot n = 0$ on $\partial\Omega$

$$\begin{cases} \int_{\Omega} u \cdot \nabla \Psi \, dx - \int_{\partial\Omega} u \cdot n \Psi \, ds = - \int_{\Omega} G^{\text{pump}} \Psi \, dx \\ \int_{\Omega} (u \cdot v + \nabla \Phi \cdot v) \, dx = 0 \end{cases}, \quad \forall (v, \Psi) \in H(\text{div}) \times L^2(\Omega)$$

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Finite Element approximation: $RT_0 \times \mathbb{P}_0$

Pros:

- Good representation of the velocity field

Cons:

- In order to assure the well-posedness of the problem, we add a perturbation term $\epsilon\Phi$ to the first equation

Approximation of gas and water concentrations

Pure advection equation using Lax-Wendroff

$$\phi \frac{\partial G}{\partial t} + u \cdot \nabla G = f(t, x)$$

Pros:

- It solves the pure advection equation

Cons:

- Some spurious numerical oscillations may appear

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Advection-diffusion equation using SUPG stabilization

$$\phi \frac{\partial G}{\partial t} + u \cdot \nabla G + k_G \Delta G = f(t, x)$$

Pros:

- It stabilizes the equation for a wide range of Péclet numbers

Cons:

- It introduces a diffusion term which is not present in the original model and requires caution handling near the boundary

1 Introduction

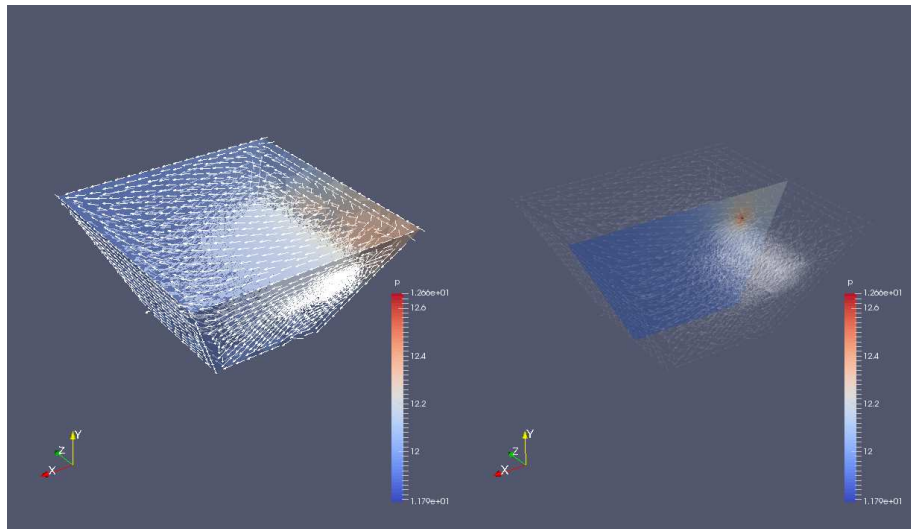
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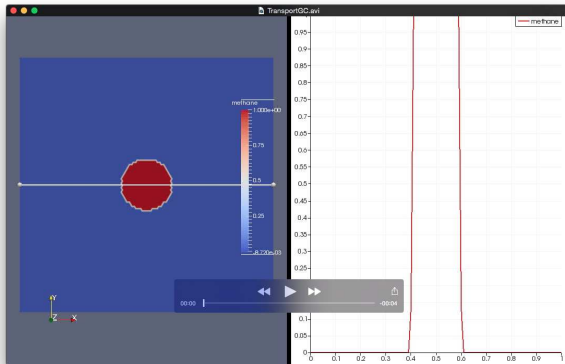
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Mixed formulation: velocity field and pressure



Velocity field and pressure computed in alveolus 7b

Advection equation 1/3



- 2D advection-diffusion equation with high Péclet number: test case without stabilization

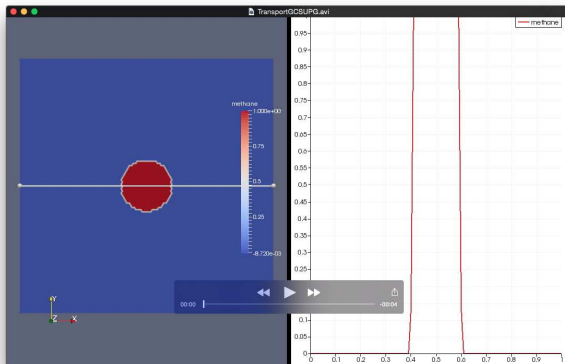


Movie Player



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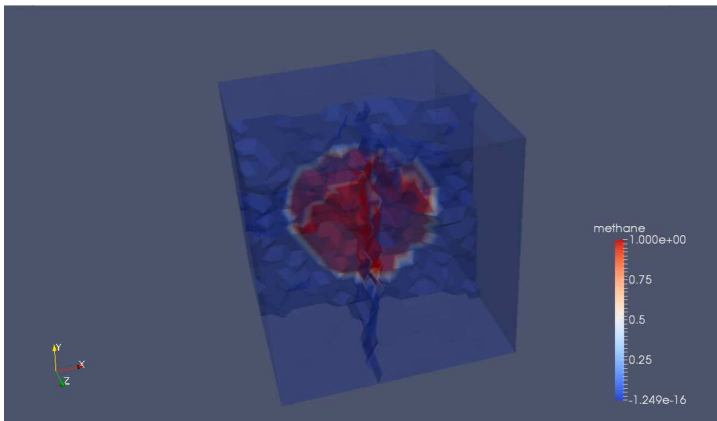
Advection equation 1/3



- 2D advection-diffusion equation with high Péclet number: test case with SUPG



Advection equation 2/3



- 3D advection-diffusion equation with high Péclet number: test case with SUPG

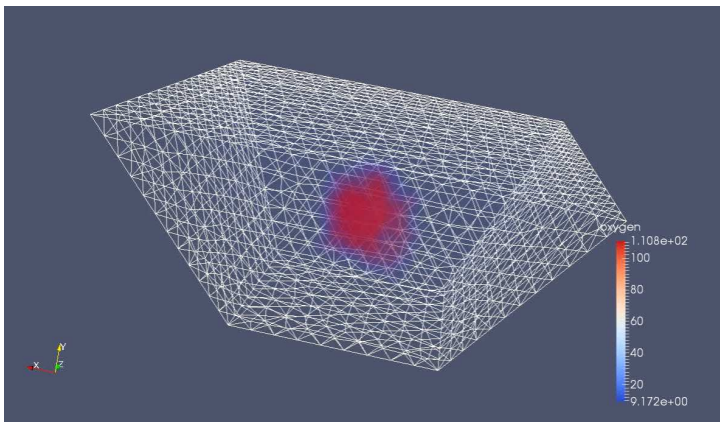


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Advection equation 3/3



- 3D pure advection equation using 1-step Lax-Wendroff method



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Conclusions

About Feel++:

- Feel++ is a very generic and rich environment for Finite Element computations
- Feel++ is highly scalable and allows applications in several fields
- Feel++ experience may be greatly improved by means of additional documentation and well-documented tutorials

About the bioreactor landfill model:

- Several numerical schemes for the simulation of a bioreactor landfill have been explored
- A partial coupling of the equations has been implemented

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What's next:

- Tune the parameters involved in each equation
- Couple the full model
- Perform data assimilation to tune the parameters of the full model
- Compute some long-time predictions of methane production

Special thanks to Christophe Prud'homme for his support and his suggestions during the development of this project.

Thanks to all the Cemracians: organizers and participants.