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SIMULATING BIOLOGICAL DYNAMICS USING PARTIAL DIFFERENTIAL EQUATIONS:

APPLICATION TO DECOMPOSITION OF ORGANIC MATTER IN 3D SOIL STRUCTURE

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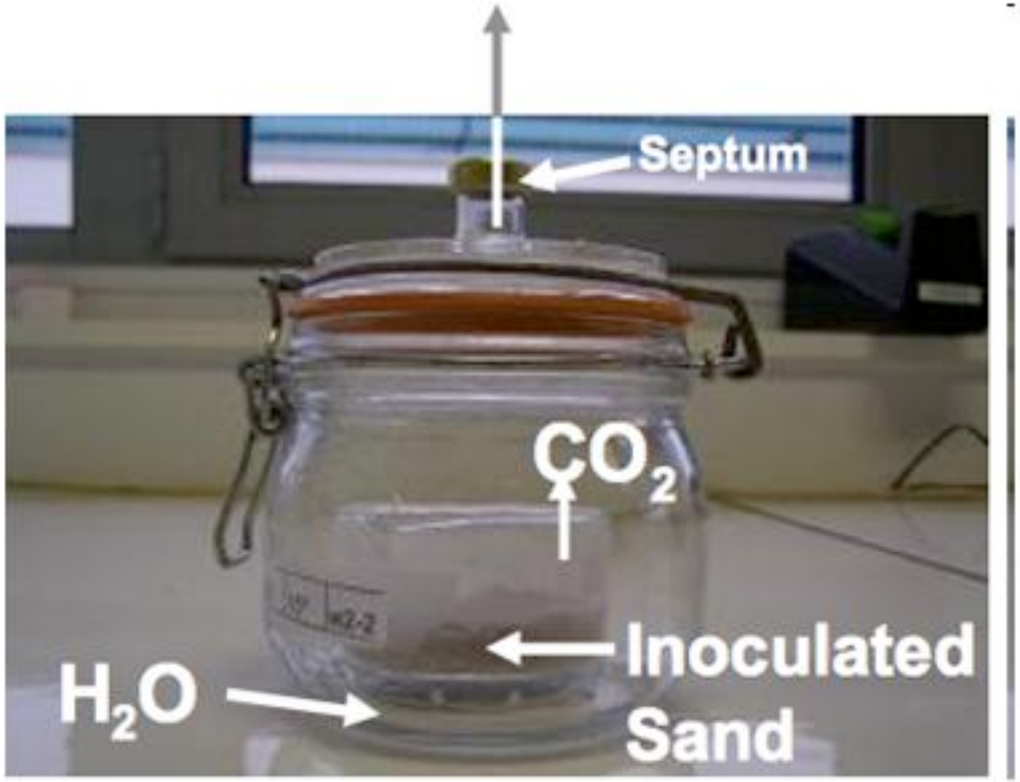
OUTLINE

- Biological problem
- PDE model
- Simulating the model
- Conclusions and Perspectives

Biological problem



T=25°C

Water content of 0.216 g H_2O / g soil

Coucheney E. ***Effets combinés de facteurs climatiques et de la diversité sur le fonctionnement de communautés bactériennes: respiration et métabolomique.*** **These doctorale Université Pierre et Marie Curie, 194 pages, 2009.**

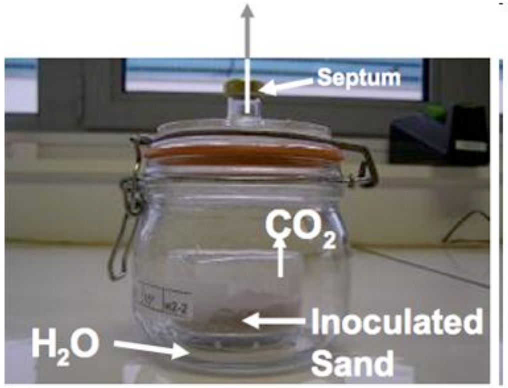
Biological problem

Input data

+ 3D soil structure

+ Initial spatial distribution of biological elements:

- Micro-organism (**MB**)
- Dissolve Organic Matter (**DOM**)
- Fresh Organic Matter (**FOM**)
- Soil Organic Matter (**SOM**)
- Enzymes (**ENZ**)
- Inorganic organic matter (**CO2**)



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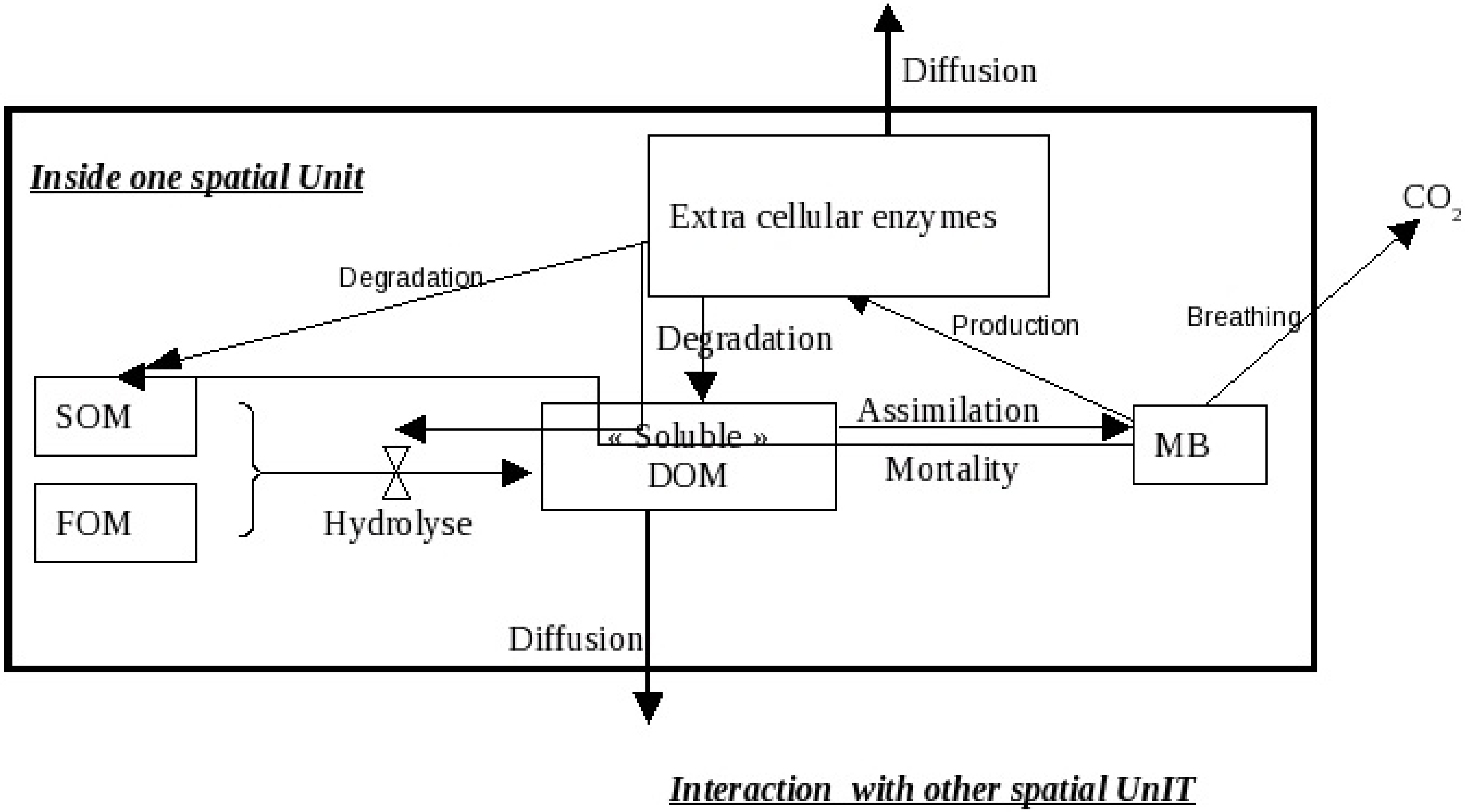
Biological problem



PDE model

Let $T > 0$ be a fixed time and let's define

$$\Omega_T = \Omega \times]0, T[.$$

$$
\begin{aligned}
\frac{\partial b}{\partial t} &= D_b \Delta b + \left(\frac{k\, n}{K_b + n} - \mu - r - \nu \right) b, \\
\frac{\partial n}{\partial t} &= D_n \Delta n + \frac{e}{K_m + e}(c_1\, m_1 + c_2\, m_2) - \frac{k\, n}{K_b + n} b + \alpha_1(\zeta) e + \alpha_2(\mu) b, \\
\frac{\partial m_1}{\partial t} &= -\frac{c_1\, e}{K_m + e} m_1 + (1 - \alpha_1(\zeta)) e + (1 - \alpha_2(\mu)) b, \\
\frac{\partial m_2}{\partial t} &= -\frac{c_2\, e}{K_m + e} m_2, \\
\frac{\partial e}{\partial t} &= D_e \Delta e + \nu\, b - \zeta\, e, \\
\frac{\partial c}{\partial t} &= D_c \Delta c + r\, b.
\end{aligned}
$$

PDE model

$$
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\frac{\partial m_1}{\partial t} &= -\frac{c_1\, e}{K_m + e} m_1 + (1 - \alpha_1(\zeta)) e + (1 - \alpha_2(\mu)) b, \\
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\frac{\partial e}{\partial t} &= D_e \Delta e + \nu\, b - \zeta\, e, \\
\frac{\partial c}{\partial t} &= D_c \Delta c + r\, b.
\end{aligned}
$$

We use Neumann homogeneous boundary conditions and the following initial conditions **in** Ω:

- $b_0(x)$ for MB,
- $n_0(x)$ for DOM,
- $m_{10}(x)$ for SOM,
- $m_{20}(x)$ for FOM,
- $e_0(x)$ for ENZ
- $c_0(x)$ for CO2.

PDE model: vector form

We simplify the system writing by transforming it into a vector form. Let's define vectors the following way:

$$\begin{aligned} u &\equiv \left(u_1, u_2, u_3, u_4, u_5, u_6\right)^t, \\ &\equiv \left(b, n, m_1, m_2, e, c\right)^t \end{aligned}$$

$$u_0 \equiv \left(b_0, n_0, m_{10}, m_{20}, e_0, c_0\right)^T.$$

The diffusion coefficients matrix $\underline{D}$ is defined as follows:

$$\underline{D} = \begin{pmatrix} D_b & 0 & 0 & 0 & 0 & 0 \\ 0 & D_n & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & D_e & 0 \\ 0 & 0 & 0 & 0 & 0 & D_c \end{pmatrix}.$$

PDE model: vector form

$$
\begin{aligned}
F_1(u) &= \Big(\frac{k\,u_2}{K_s+u_2}-\mu-r-\nu\Big)u_1,\\
F_2(u) &= \frac{k\,u_5}{K_m+u_5}\Big(c_1\,m_1+c_2\,m_2\Big)-\frac{k\,u_2}{K_s+u_2}u_1+\alpha_1(\zeta)u_5+\alpha_2(\mu)u_1,\\
F_3(u) &= -\frac{c_1u_5}{K_m+u_5}u_3+(1-\alpha_1(\zeta))u_5+(1-\alpha_2(\mu))u_1,\\
F_4(u) &= -\frac{c_2u_5}{K_m+u_5}u_4,\\
F_5(u) &= \nu u_1-\zeta u_5,\\
F_6(u) &= ru_1.
\end{aligned}
$$

Let's define the vector function F such that

$$F(u)=(F_1(u),F_2(u),F_3(u),F_4(u),F_5(u),F_6(u))^T.$$

PDE model: vector form

The vector form of the system is given by:

$$\begin{cases} \partial_t u & = & \operatorname{div}\big(\underline{D}\nabla u\big) + F(u) & \text{in } \Omega_T, \\ \frac{\partial u}{\partial n} & = & 0 & \text{on } \partial\Omega \times]0, T[, \\ u(t=0) & = & u_0 & \text{in } \Omega. \end{cases}$$

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Domain: definition of pore space

Geoscience

A **pore** is usually defined as a **cavity filled with fluids** (air or water)

Vogel, H.J., Roth, K.I., 2001. Quantitative morphology and network representation of soil pore structure. Advances in Water Resources 24 (3), 233–242.

Pore space is commonly understood as a **set of pores**

Geometrical definition

Definition 1. :

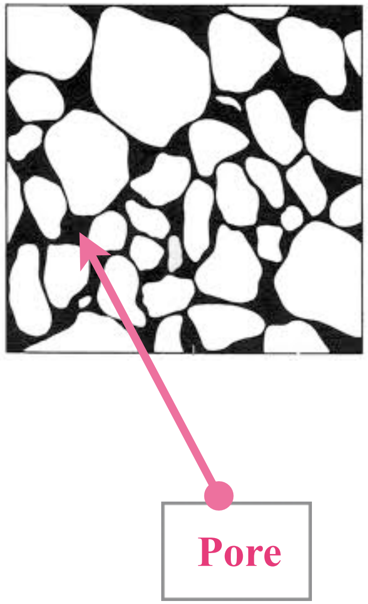
Let p be the pore space defined by its indicative function I.

Let $M(i,j,k)$ be a point of the 3D affine space whose coordinates are (i,j,k).

We have

$$M(i,j,k) \in p \Leftrightarrow I(i,j,k) = 1 \quad (1)$$

From a practical point of view, when pore space is extracted from a computed tomography image, the function I is directly defined by the result of the image thresholding. In this case, each point (i,j,k) is attached to a voxel.



Monga, O., Ngom, N.F., Delerue, J.F., 2007. Representing geometric structures in 3D tomography soil images: application to pore space modelling. Computers & Geosciences 33, 1040–1161.

Domain: Maximal ball

Definition 2. :

Let $B(C,r)$ be an open ball included in p whose centre is C and whose radius is r

$$B(C,r) \subset p \tag{2}$$

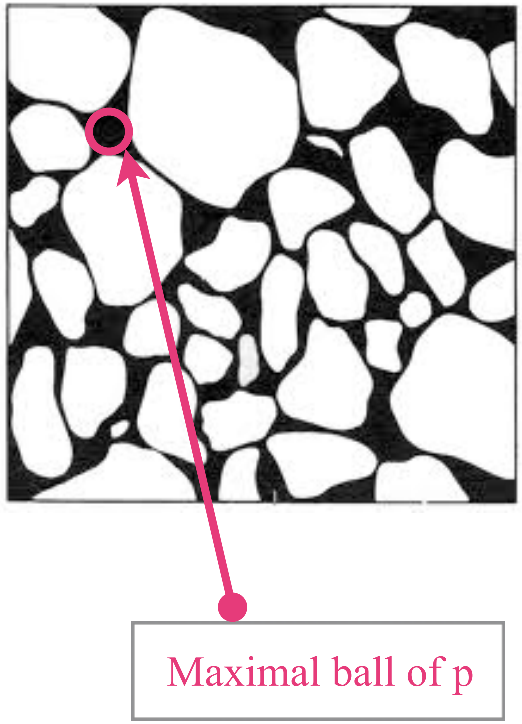
We consider that $B(C,r)$ is a maximal ball of p if and only if

$B(M,s)$ refers to any open ball whose centre is M and whose radius is s.

$$\forall B(M,s)/B(M,s) \subset p; \quad B(C,r) \subset B(M,s) \Rightarrow B(M,s) = B(C,r) \tag{3}$$

$B_{\max}(p)$ is the set of all maximal balls of pore space p.

This means that a maximal ball of pore space p is a ball that cannot be contained by any other ball in p.



Domain: Skeleton

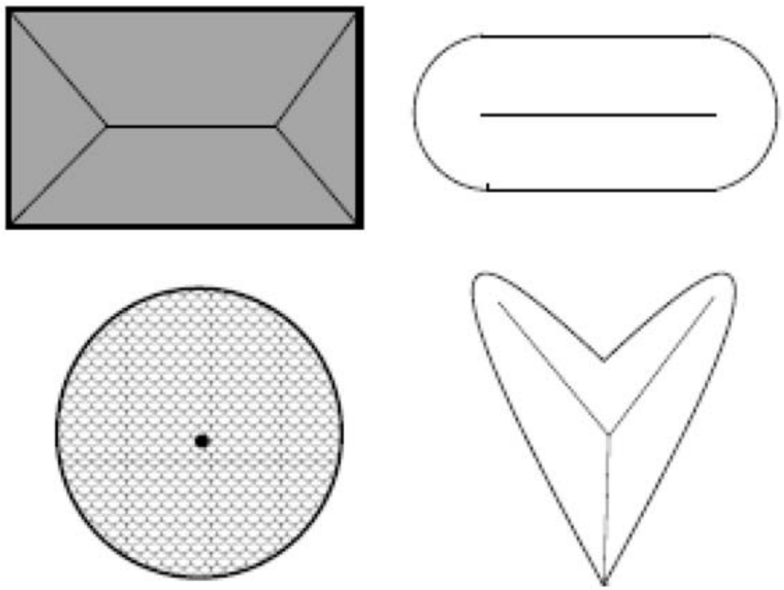
Definition 3. :

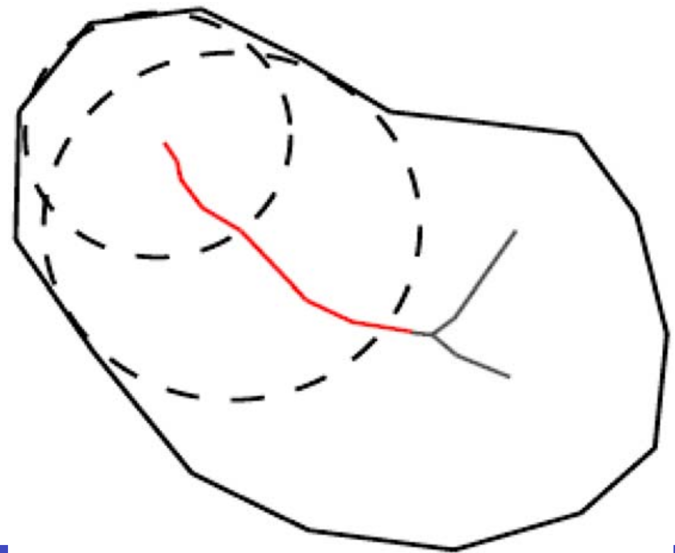
The skeleton of p (S_p) is defined as the set of the centres of all maximal balls (Attali et al., 2007; Schmitt and Mattioli, 1994)

$$M \in S_p \Leftrightarrow \exists B(M, r) \in B_{\max} \quad (4)$$

Attali, D., Boissonnat, J.-D., Edelsbrunner, H., 2007. Stability and computation of medial axes: a state of the art report. In: Hamann, B., Moller, T., Russell, B. (Eds.), Mathematical Foundations of Scientific Visualization, Computer Graphics, and Massive Data Exploration. Mathematics and Visualization Series. Springer /http://www.lis.inpg.fr/pages_perso/attali/publications.htmlS.

Schmitt, M., Mattioli, J., 1994. Morphologie Mathe´matique (Mathematical morphology). Masson, Paris, 228 p.





Domain: Finite recovering

Definition 4 ((*new*)). Let A be a set of maximal balls of p. We define $R(p)$ as the finite set of maximal balls recovering the skeleton

$$R(p) = \{A \subset B_{\max}(p)/((S_p \subset A)\Lambda(\text{Card}A) < +\infty))\} \quad (5)$$

The union of all maximal balls forms the shape. We choose to describe the shape by a minimal set of maximal balls recovering the shape skeleton. This minimal set provides a shape approximation that preserves the shape topology and accurately describes shape cavities (Monga et al., 2007).

Monga, O., Ngom, N.F., Delerue, J.F., 2007. Representing geometric structures in 3D tomography soil images: application to pore space modelling. Computers & Geosciences 33, 1040–1161.

Theorem1 ((*new*)). *If the skeleton of p (S_p) is a compact set, then*

$$R(p) \neq \varnothing \quad (6)$$

Domain: Minimum skeleton recovering

Conjecture 6 ((*new*)). *In most cases, the skeleton of a shape can be approximated by a compact set. This issue will be discussed in more detail in a forthcoming paper. We can therefore consider that from a practical point of view, the skeleton can always be recovered by a finite set of maximal balls.*

Definition 5 ((*new*)). Let K and H be sets of maximal balls recovering the skeleton. We define $R_{\min}(p)$ as the element of $R(p)$ with a minimal cardinal, that is

$$R_{\min}(p) = \{K \in R(p)/(\forall H \in R(p), \mathrm{Card}(K) \leqslant \mathrm{Card}(H))\} \quad (9)$$

$R_{\min}(p)$ then contains all minimal recoveries of the skeleton of p by maximal balls.

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Domain: Definitions with scale factor

Definition 6 ((*new*)). If we consider the λ-skeleton instead of the skeleton itself, Definition 5 can be directly generalised. The λ-skeleton (Chazal and Lieuthier, 2005) can be considered as all centres of maximal balls whose radius is at least λ. We can therefore extend the above definitions to obtain the notion of $R_{\min,\lambda}(p)$ corresponding to the minimal recovery of the λ-skeleton of p using maximal balls with a radius of more than λ. $R_{\min,\lambda}(p)$ is an accurate way to simply define pore space at different scales. In the following, we will refer to $R_{\min}(p)$ as MIRES(p) and to $R_{\min,\lambda}(p)$ as λ_MIRES(p). By doing this, we generalise Definition 5 by adding a scale factor.

Chazal, F., Lieuthier, A., 2005. The lambda medial axis. Graph Models 67 (4), 304–331.

Algorithm

Computation of a minimal set of maximal balls recovering the pore space skeleton

Algorithm:

Extraction of maximal balls and the λ-skeleton using 3D Delaunay triangulation

- Computation of the volume shape border: 26-connectivity
- Computation of 3D Delaunay triangulation of the volume shape border

Frey, P.J., 2001. MEDIT: an interactive visualization software. INRIA Technical Report 0253, INRIA (Instiut National de Recherche en Informatique et Automatique), Rocquencourt, France, 41p.

George, P.L., 2004. Tetmesh-GHS3D, Tetrahedral mesh generator. INRIA User's Manual, INRIA (Institut National de Recherche en Informatique et Automa- tique), Rocquencourt, France, 13 p.

George, P.L., Borouchaki, H., 1998. Delaunay Triangulation and Meshing. Hermes, Paris, 413 p (ISBN 2-86601-692-0).

- Computation of Delaunay spheres
- Pruning of Delaunay spheres
- Computing the λ-skeleton

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Algorithm:

From maximal balls to minimum skeleton recovery

I. Set φ to NIL; where φ is the final list of spheres.
II. INTMAX = 0.
III. Enter a list S all Delaunay spheres included within the shape with a radius of at least λ, not included in list φ, and which are not marked.
IV. If S is empty, go to XII.
V. Sort all spheres of S according to their radius in decreasing order.
VI. Take out the head of S that is the sphere with the highest radius. This sphere will be referred to as T.
VII. If S is empty, go to XII
VIII. Compute the intersection of T with all spheres of φ. For each intersection, compute the ratio between the intersection volume and the minimum of the volumes of the two spheres. Compute the maximal value for this ratio, which will be referred to as $R_{\max}(T)$.
IX. If $R_{\max}(T)$ is less than a given threshold INTMAX, then put T in the list φ and go to III.
X. If $R_{\max}(T)$ is greater than INTMAX, then mark T and go to VI.
XI. If S is not empty, go to IV.
XII. If the union of spheres (balls) of φ includes all points of the λ-skeleton, the process is terminated.
XIII. INTMAX = INTMAX+0.1.
XIV. Go to II.

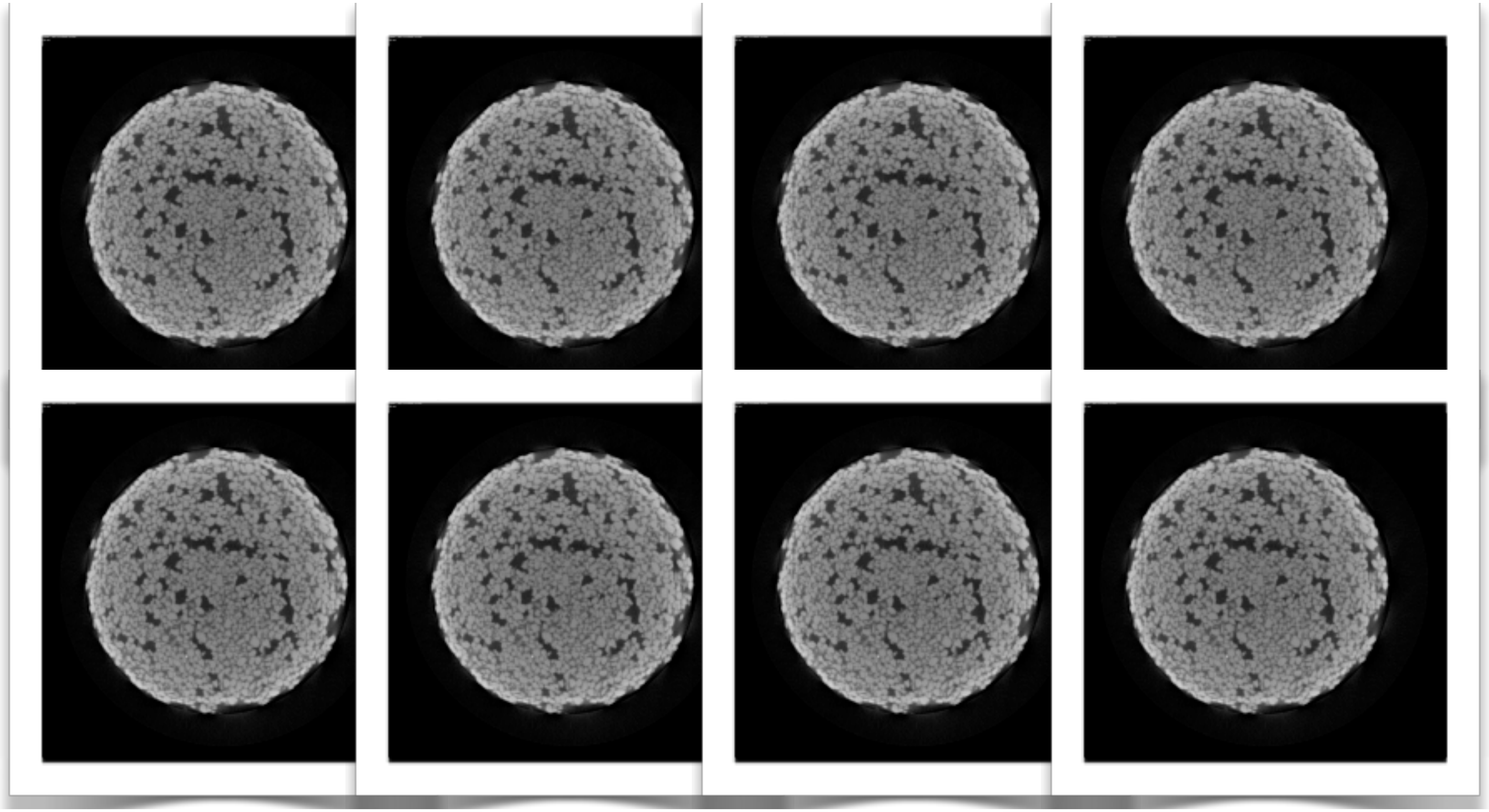


Fig. 1 bis: Successive slices (1650 x 1650) of CT image of a sand soil sample

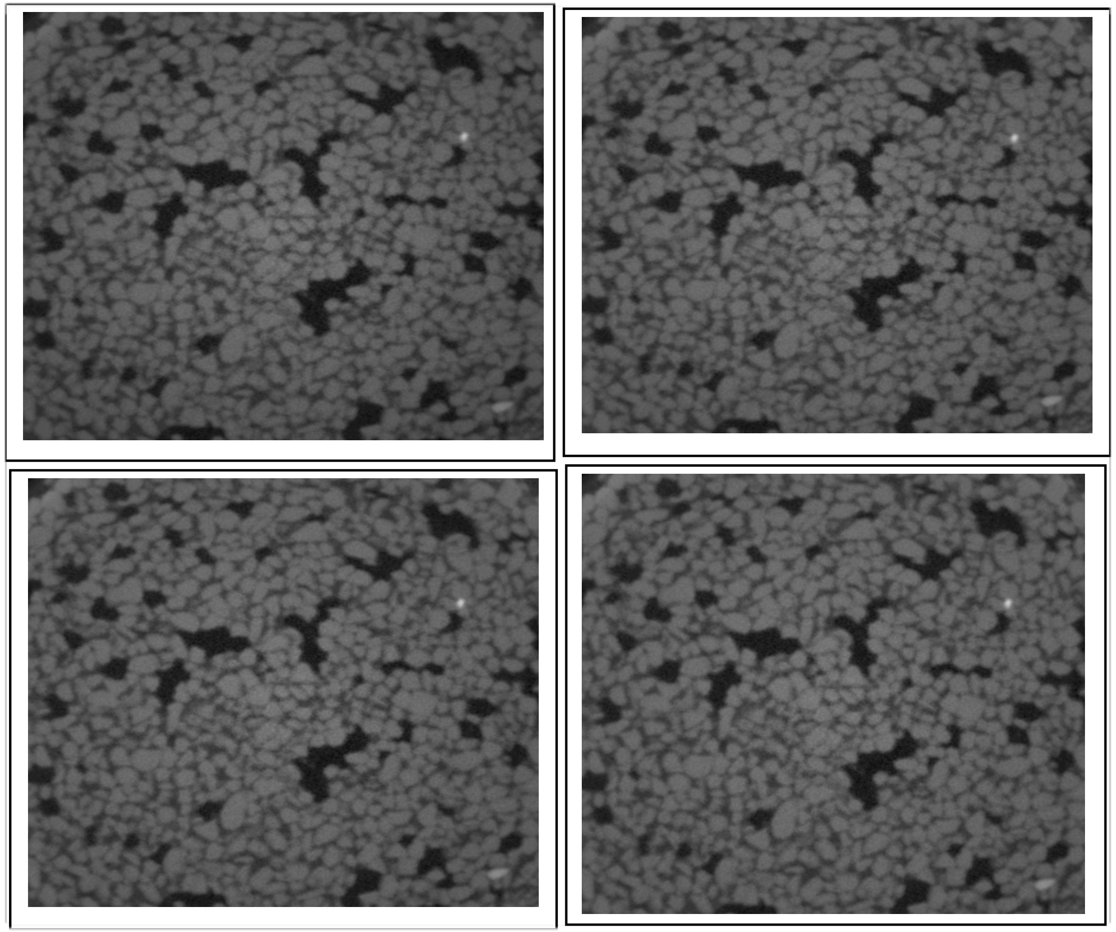


Fig. 2bis: successive slices (400 x 400) of the (400 x 400 x 400) 3D image extracted

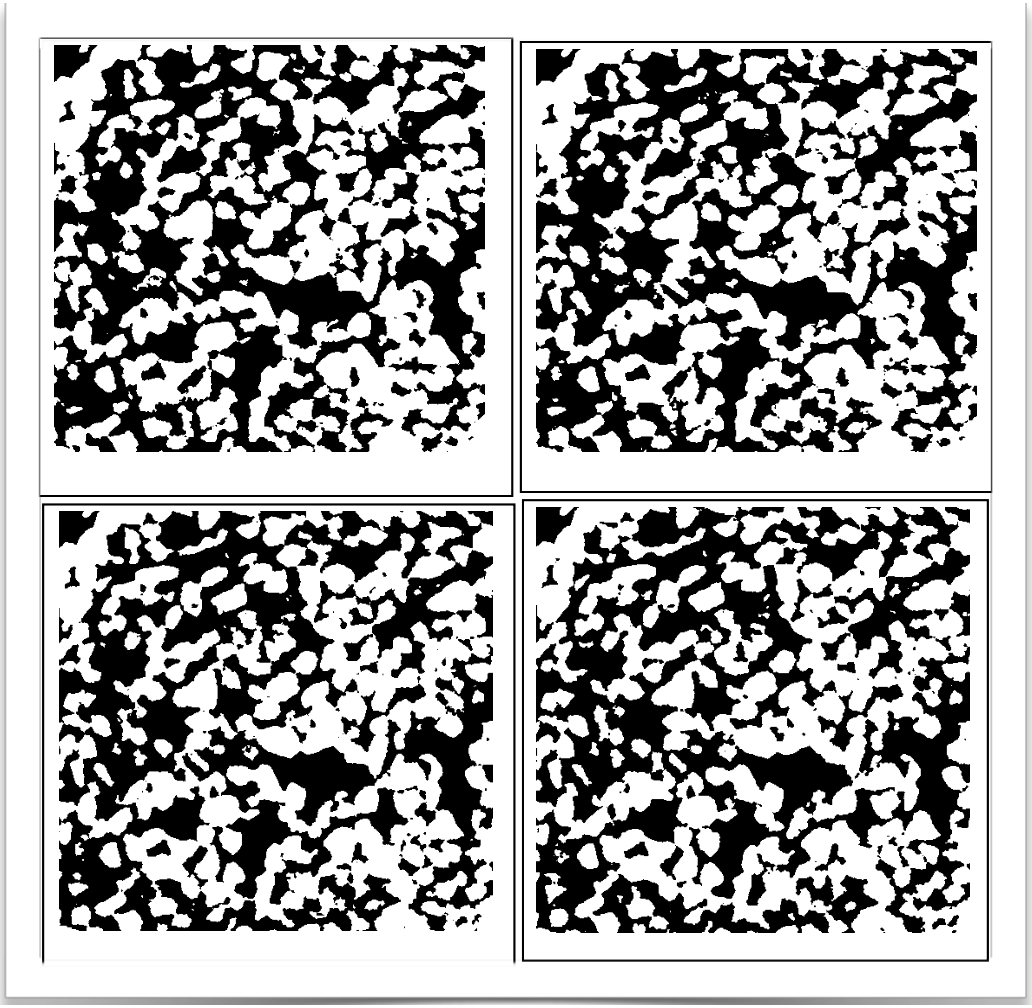


Fig. 3bis: cross section representing pore space (white color), the porosity is 35%.

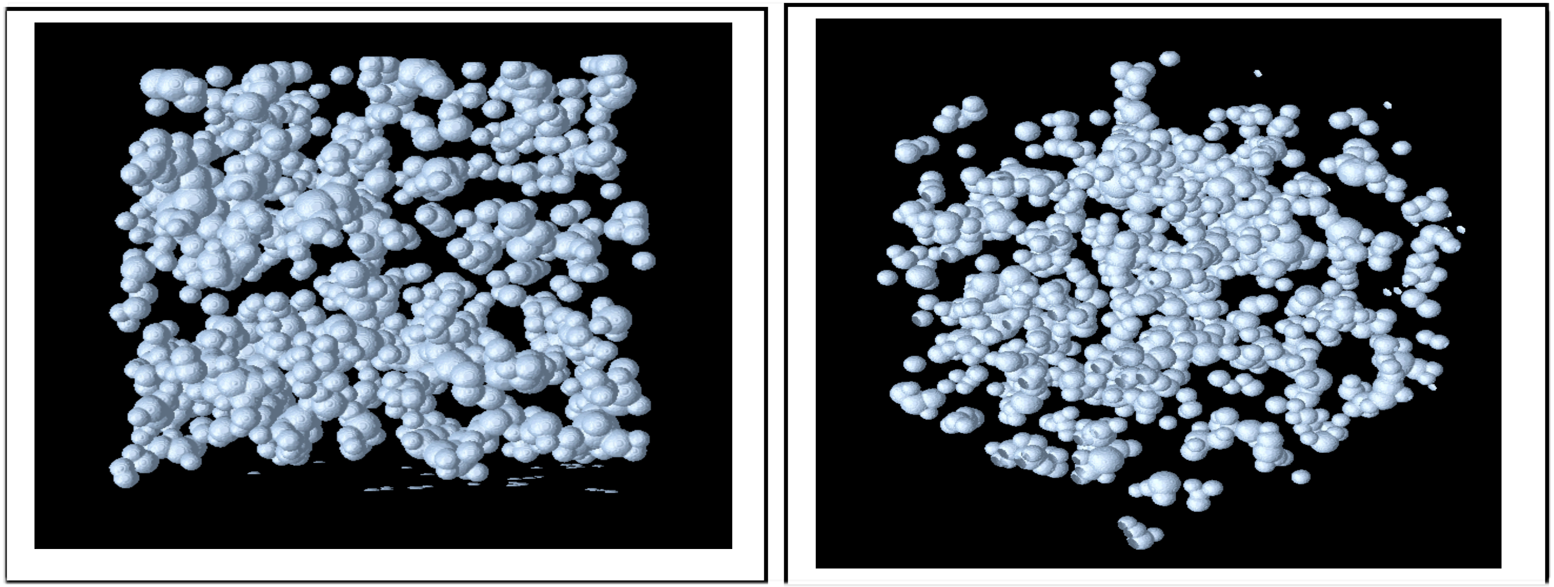
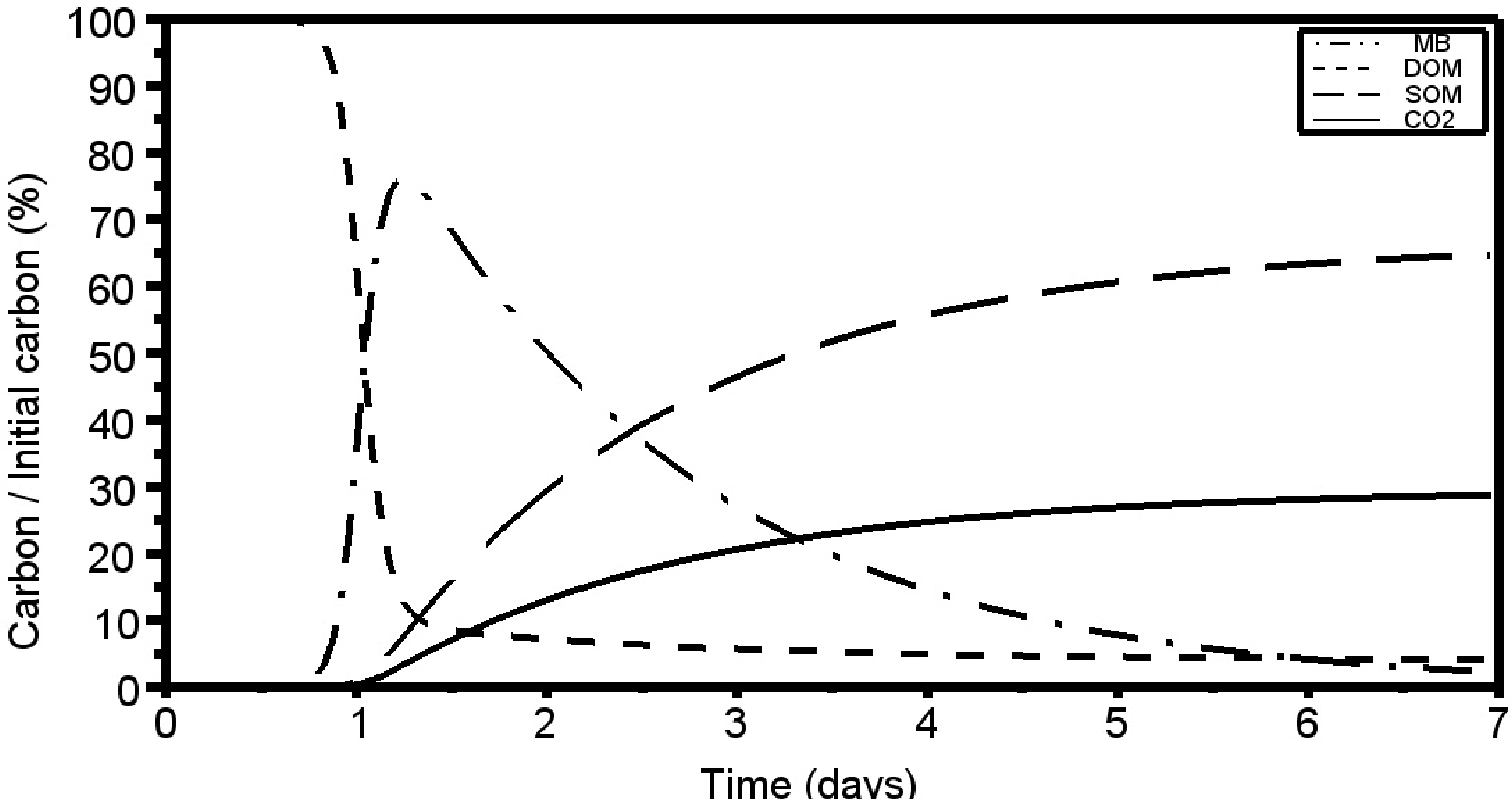
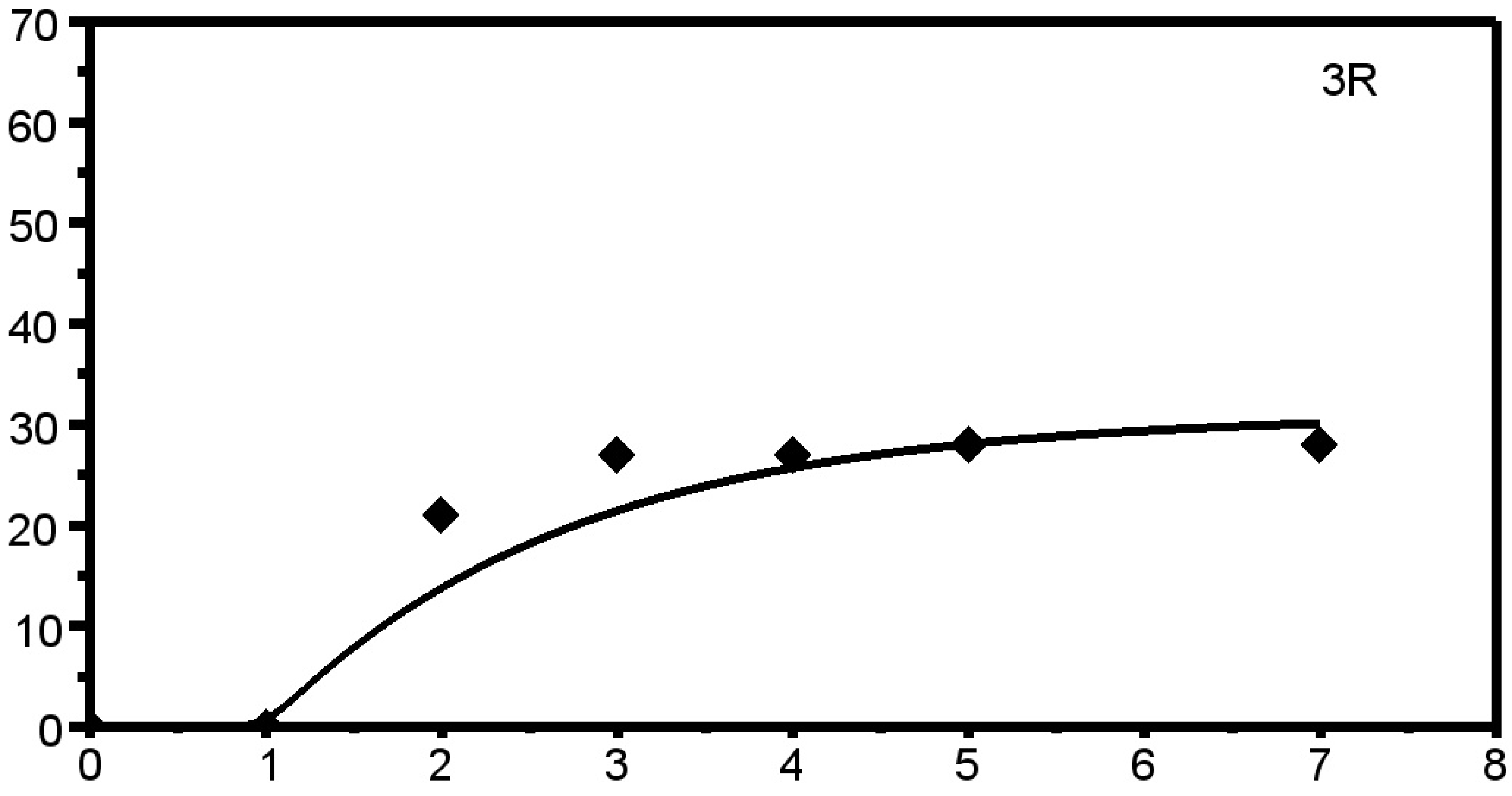


Fig. 4bis: perspective views of the ball based pore space representation, we display only the balls whose radius is at leat 10

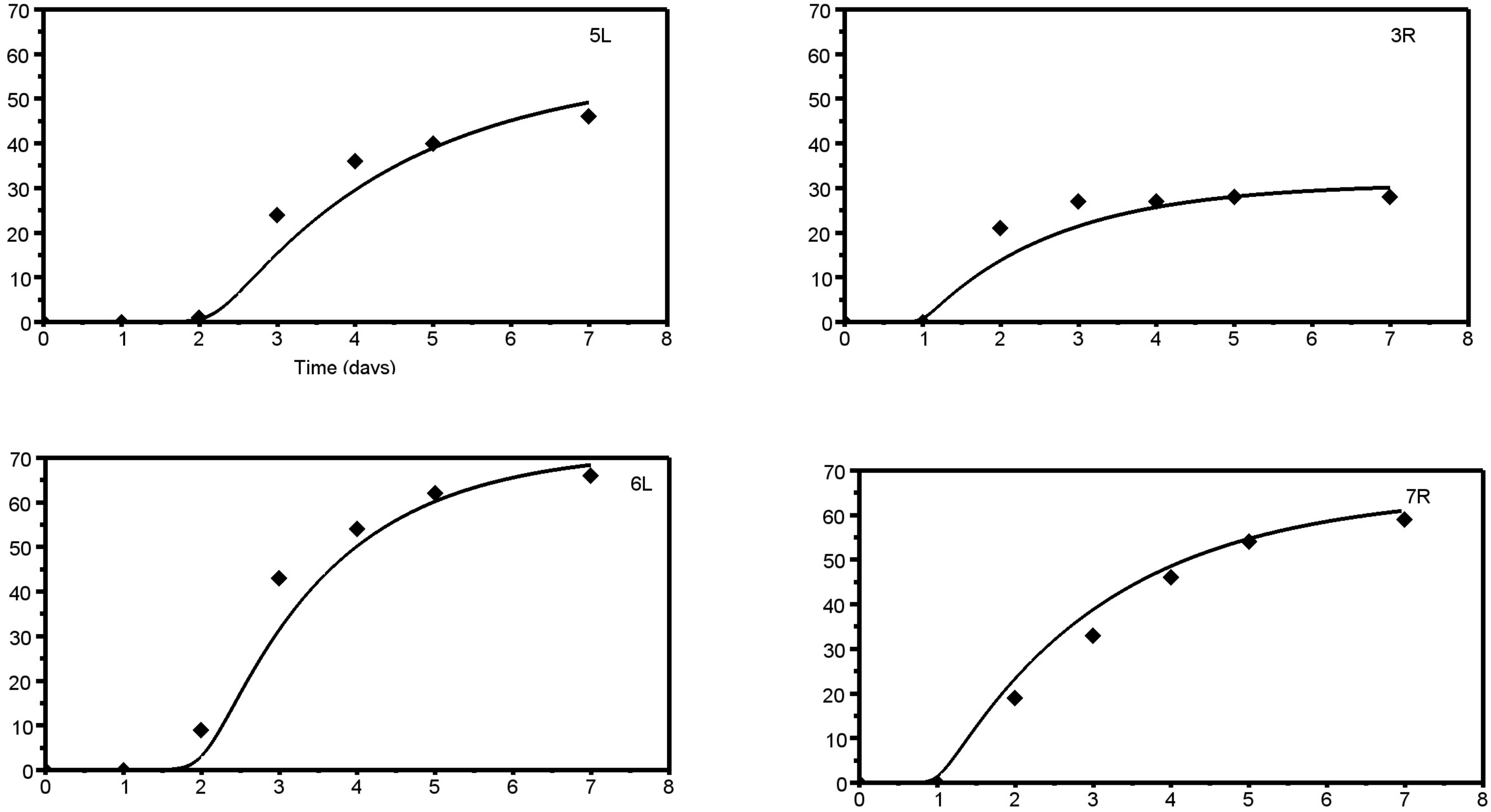
Simulation: 3R



Simulation: 3R



Simulation



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Conclusions and perspectives

- Using PDE modeling approach in order to simulate the biological system.
- Investigate the quality properties of the model
- Generating more complicated models to the biological system
- Other biological systems...

Thanks

Thank you very much for your attention!