Presented at the COMSOL Conference 2008 Boston

COMSOL CONFERENCE BOSTON 2008

Transport, Growth, Decay and Adsorption of Microorganisms and Nutrients through Porous Media:

A Simulation with COMSOL

D.A. López Falcón, M.A. Díaz Viera & A. Ortiz Tapia

Programa de Recuperación de Hidrocarburos
del Instituto Mexicano del Petróleo (IMP)

IMP
INSTITUTO MEXICANO DEL PETRÓLEO

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Motivation

- *We are interested in model and simulate the fate of microorganisms in porous media, which is a very important, complex and interacting phenomenon; mainly because it involve living entities.*
- *The systematic modeling approach to continuum systems [1], allow us to derive a model including as many constitutive laws as we need to describe even the most complex phenomena.*
- *COMSOL Multiphysics [2], provide us with a multifunctional and general framework as well as useful application modes to implement our model.*

[1] Allen et al. "Numerical modeling in science and engineering", John Wiley & Sons., USA, (1988)

[2] COMSOL Multiphysics, Earth Science Module, User's Guide Version 3.3, 37, COMSOL LAB (2006)

Background

- *In spite of that there are some models proposed in the literature for the transport of microorganisms in porous media [3-5], we derive our model and perform a procedure to set it up, with the intend to achieve more insight about the problem.*
- *In all these above mentioned references, the transport model has been implemented using Finite Difference Methods; evidently our COMSOL implementation is solved using Finite Element Methods.*

[3] Tan et al. "Transport of bacteria in an aquifer sand: Experiments and model simulations", Water Resources Research, 30 (12), 3243-3252, (1994)

[4] Sen et al. "Bacterial transport in porous media: New aspects of the mathematical model", Colloids and Surfaces, A 260, 53-62, (2005)

[5] Chang et al. "Modeling and Laboratory Investigation of Microbial Transport Phenomena in Porous Media", SPE 22845, (1991)

The model (1)

The local balance equation of the intensive property ψ_γ^α *is the PDE [1]:*

$$\frac{\partial \psi_\gamma^\alpha}{\partial t} + \nabla \cdot \left(\psi_\gamma^\alpha \vec{v}^\alpha - \vec{\tau}_\gamma^\alpha \right) = g_\gamma^\alpha; \quad \forall \vec{x} \in B(t)$$

where $\vec{v}^\alpha$ *is the velocity of the phase,* $\vec{\tau}_\gamma^\alpha$ *is the flux field through the boundary, and* g_γ^α *is the generation into the body.*

Phase (α)	Component (γ)	Intensive Property ψ_γ^α
Water (w)	Water (w)	$\phi\rho_w$
	Planktonic (pm)	ϕc_{pm}^w
	Nutrients (n)	ϕc_n^w
Biofilm (b)	Sessile (sm)	$c_{sm}^b = \rho_m \sigma$
Solid (s)	Rock (r)	$\rho_{r_b} = (1-\phi)\rho_{r_p}$
	Nutrients (n)	$\rho_{r_b} c_n^s$

Table 1: Intensive properties associated with mass of components

Here ϕ *is the porosity,* ρ *represent mass densities, c denotes concentrations and* σ *is the volume of sessile microorganisms by unit volume of bulk porous media.*

The model (2)

The mass local balance equation of the planktonic microorganism is:

$$\frac{\partial}{\partial t}\left(\phi c_{pm}^{w}\right)+\nabla\cdot\left(\phi c_{pm}^{w}\vec{v}^{t}-\mathbf{D}_{pm}^{w}\cdot\nabla\left(\phi c_{pm}^{w}\right)\right)=\left(\mu-k_{d}-k_{a}\right)\phi c_{pm}^{w}+k_{r}\rho_{m}\left(\sigma-\sigma_{irr}\right)$$

where the total velocity is composed by adding mean water, chemotactic, and sedimentation velocities, i.e. $\vec{v}^{t}=\vec{v}^{w}+\vec{v}^{c}+\vec{v}^{g}$*;*

the dispersion tensor is $\mathbf{D}_{pm}^{w}$*,*

the Monod specific growth rate is μ *,*

the cell's specific decay rate is k_{d}*,*

the adsorption rate coefficient is k_{a}*,*

the desorption rate coefficient is k_{r}*,*

and the minimum volume of sessile cell fraction is σ_{irr} *.*

The model (3)

The mass local balance equation of the sessile microorganism is:

$$\frac{\partial}{\partial t}\left(\rho_m\sigma\right)=\left(\mu-k_d-k_r\right)\rho_m\sigma+k_a\phi c_{pm}^w+k_r\rho_m\sigma_{irr}$$

remember that the desorption term exists only if $\sigma>\sigma_{irr}$.

The total mass local balance equation of the nutrient is:

$$\left(\phi+\rho_{r_b}\partial_{c_n^w}c_n^s\right)\frac{\partial}{\partial t}c_n^w+\nabla\cdot\left(\vec{u}^w c_n^w-\mathbf{D}_n^w\cdot\nabla\left(\phi c_n^w\right)\right)=-\mu\left(\phi c_{pm}^w+\rho_m\sigma\right)/Y_{m/n}$$

select one of the predefined adsorption isotherm.

The model (4)

The initial conditions are:

$$c^{w}_{pm}\Big|_{t=0} = \sigma\Big|_{t=0} = c^{w}_{n}\Big|_{t=0} = 0$$

The inlet boundary condition (general) is:

$$-\hat{n}\cdot\left[\phi c^{w}_{\gamma}\vec{v} - \mathbf{D}^{w}_{\gamma}\cdot\nabla\left(\phi c^{w}_{\gamma}\right)\right]\Big|_{x=0} = \hat{n}\cdot\phi c^{w}_{\gamma_0}\vec{v}$$

where $\gamma = pm, n$ *and* $c^{w}_{\gamma_0} \neq 0$ *only during pulse injection, i.e., for* $0 < t < t_{inj}$

The outlet boundary condition (advective flux) is:

$$-\hat{n}\cdot\left[-\mathbf{D}^{w}_{\gamma}\cdot\nabla\left(\phi c^{w}_{\gamma}\right)\right]_{x=x_L} = 0$$

as above $\gamma = pm, n$.

COMSOL implementation (1)

The non-conservative form of the governing equation for saturated media available in the Solute Transport application mode of COMSOL Multiphysics is as follows [2]:

$$\theta_s \frac{\partial c_i}{\partial t} + \rho_b \frac{\partial c_{Pi}}{\partial c} \frac{\partial c_i}{\partial t} + \nabla \cdot \left(-\theta_s D_{Li} \nabla c_i \right) = -\mathbf{u} \cdot \nabla c_i + R_{Li} + R_{Pi} + S_{ci}$$

which is used to implement the mass local balance equations of the planktonic microorganism and nutrient, whereas the coefficient form of the PDE mode is used to implement the mass local balance equation of the sessile microorganism.

[2] COMSOL Multiphysics, Earth Science Module, User's Guide Version 3.3, 37, COMSOL LAB (2006)

COMSOL implementation (2)

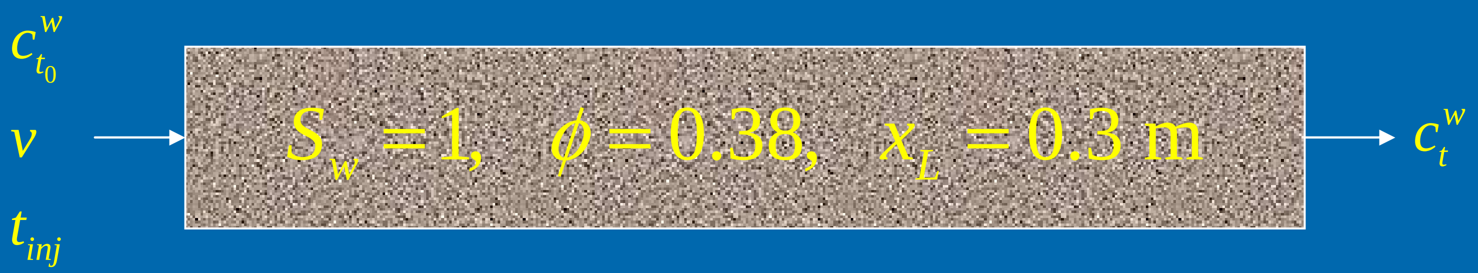
The predefined boundary conditions for solute transport are [2]:

$c_i = c_{i,0}$	Concentration
$\mathbf{n}\cdot\left(\theta_s D_{Li}\nabla c_i - \mathbf{u}c_i\right) = N_{i,0}$	Flux
$\mathbf{n}\cdot\left(\theta_s D_{Li}\nabla c_i - \mathbf{u}c_i\right) = 0$	No Flux
$\mathbf{n}\cdot\left(\theta_s D_{Li}\nabla c_i - \mathbf{u}c_i\right) = \mathbf{n}\cdot\mathbf{u}c_{i,0} + N_{i,0}$	General
$\mathbf{n}\cdot\left(\theta_s D_{Li}\nabla c_i\right) = 0$	Advective flux

We use the general and the advective flux ones, although the concentration one is used too, to make a comparison.

[2] COMSOL Multiphysics, Earth Science Module, User's Guide Version 3.3, 37, COMSOL LAB (2006)

Tracer in sandy column (1)



$c^w_{t_0}$

v → $S_w = 1, \quad \phi = 0.38, \quad x_L = 0.3\ \text{m}$ → c^w_t

t_{inj}

- ✓*A column packed with aquifer sand.*
- ✓*The fluids are injected at constant flow velocities.*
- ✓*The sand column was saturated with sterile deionized water prior to obtain the breakthrough curve (BTC).*
- ✓*A BTC is a graph of the relative concentration versus time.*

[3] Tan et al. "Transport of bacteria in an aquifer sand: Experiments and model simulations", Water Resources Research, ***30 (12),*** *3243-3252, (1994)*

Tracer in sandy column (2)

Objective: To obtain the dispersion coefficient, D.

The mass local balance equation of the tracer is:

$$\frac{\partial}{\partial t}\left(\phi c_t^w\right)+\nabla\cdot\left(\phi c_t^w\vec{v}-\mathbf{D}_t^w\cdot\nabla\left(\phi c_t^w\right)\right)=0$$

Porosity	$\phi = 0.38$
Water velocities	$v = 0.05,\ 0.1,\ 0.2\ mm/s$
Tracer injected concentration	$c_{t_0}^w = 0.01\ mol/L$
Injection time	$t_{inj} = 1\ h$
Column length	$x_L = 0.3\ m$

Table 2: Input data for tracer BTCs in sandy column [3]

Tracer in sandy column (3)

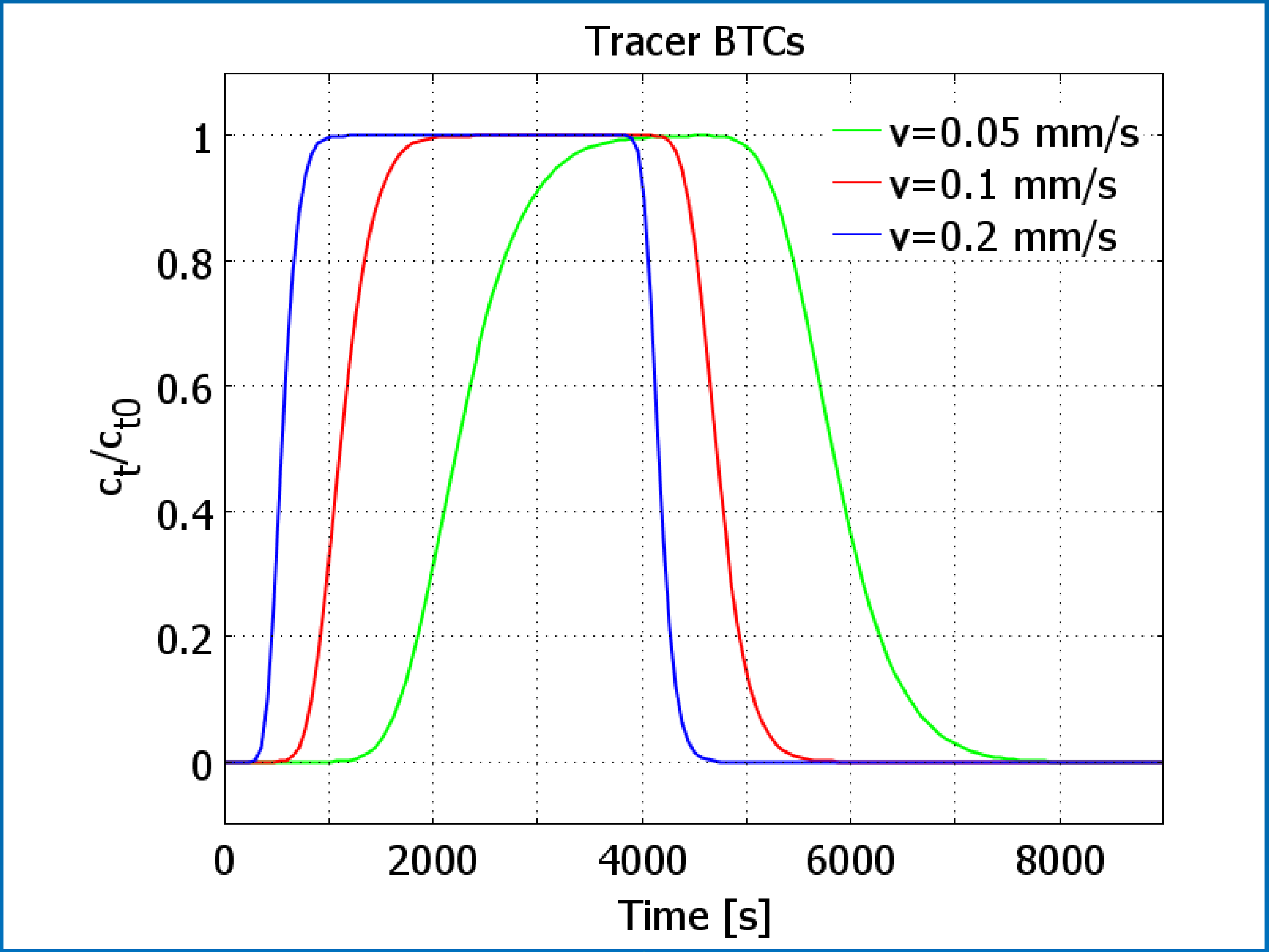
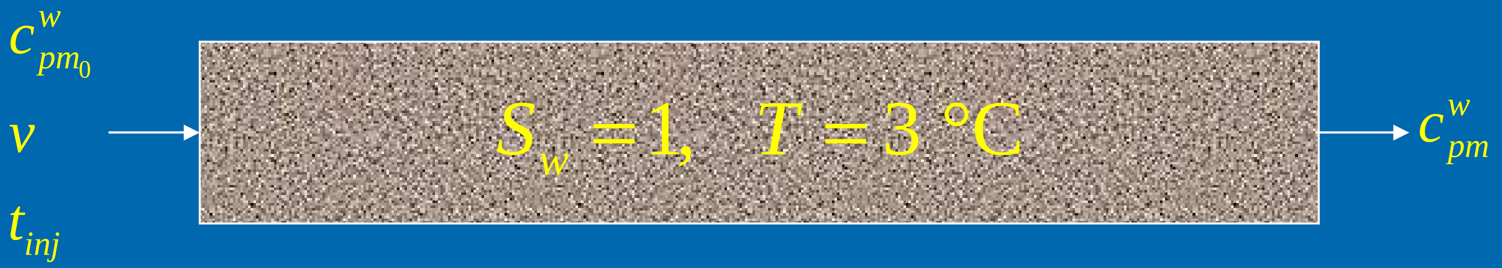


Figure 1: BTCs of sodium chloride

$$D_t^w = 1,\ 2,\ 4\ mm^2/s$$

*[4] Sen et al. “Bacterial transport in porous media: New aspects of the mathematical model”, Colloids and Surfaces, **A 260**, 53-62, (2005)*

Microorganisms transport (1)



$c^{w}_{pm_0}$

v

t_{inj}

$S_w = 1, \quad T = 3\ °C$

c^{w}_{pm}

Besides of the previous experiment conditions, we have now:

- ✓*Once porous media saturation has been achieved, the suspension of microorganisms is injected for 1 hour.*
- ✓*Then the flow of sterile deionized water was resumed.*
- ✓*The experiments were conducted at low temperature to prevent growth and death of microorganisms.*

Microorganisms transport (2)

Goal: To fit the adsorption and desorption coefficients, k_a & k_r
To compare models with varying features.

The mass local balance equation of the planktonic microorganism is:

$$\frac{\partial}{\partial t}\left(\phi c^{w}_{pm}\right)+\nabla\cdot\left(\phi c^{w}_{pm}\vec{v}-\mathbf{D}^{w}_{pm}\cdot\nabla\left(\phi c^{w}_{pm}\right)\right)=-k_a\phi c^{w}_{pm}+k_r\rho_m\left(\sigma-\sigma_{irr}\right)$$

The mass local balance equation of the sessile microorganism is:

$$\frac{\partial}{\partial t}\left(\rho_m\sigma\right)=-k_r\rho_m\left(\sigma-\sigma_{irr}\right)+k_a\phi c^{w}_{pm}$$

Dispersion coefficient	$D^{w}_{pm}=D^{w}_{t}=4$ mm²/s
Water velocity	$v=0.2$ mm/s
Microbial injected concentration	$c^{w}_{pm_0}=1.2\times10^{8}$ cells/mL
Minimum adsorbed sessile cell	$\sigma_{irr}=0.02$

Table 3: Input data for microbial BTCs in sandy column [3, 4]

Microorganisms transport (3)

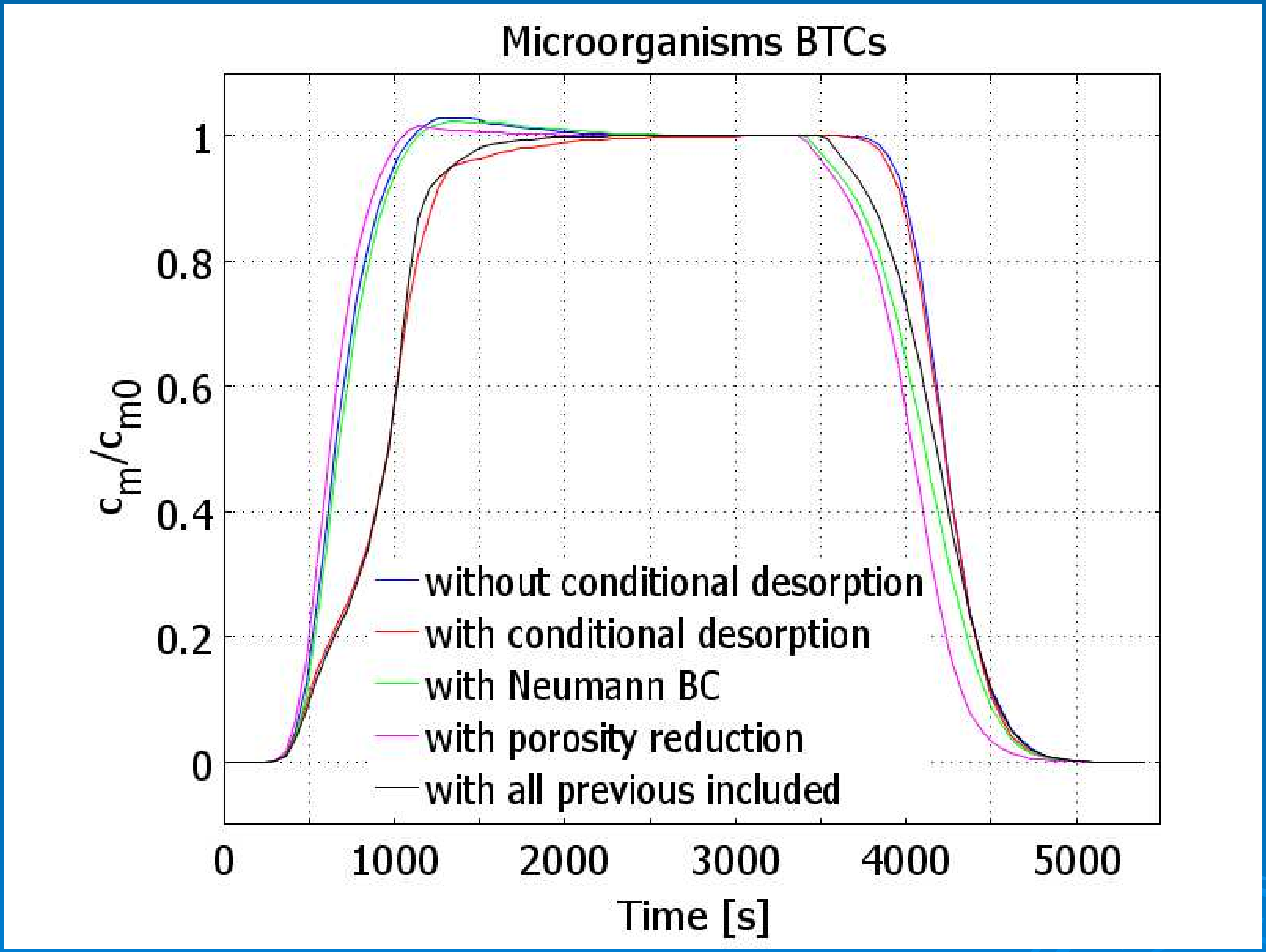


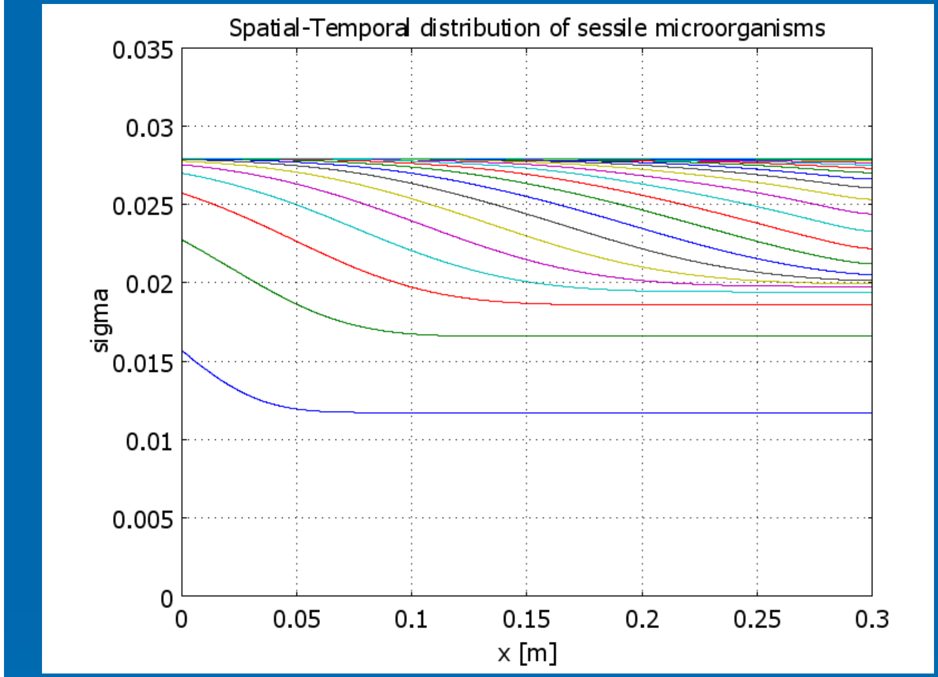
Figure 2: BTCs of microorganisms

$$k_a = 9.94\ h^{-1}$$
$$k_r = 52.94\ h^{-1}$$

Microorganisms Transport (4)

Without conditional desorption

With conditional desorption



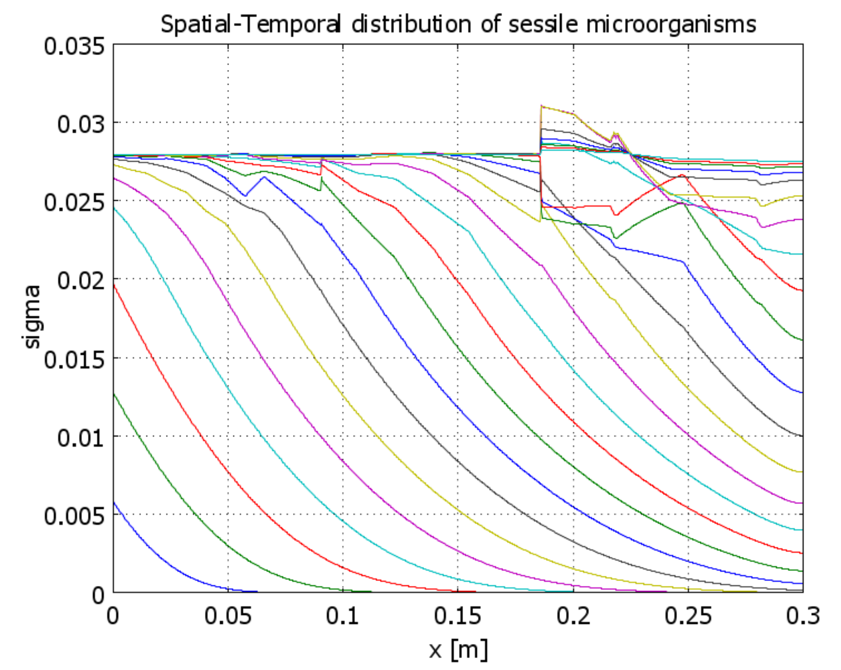


Figure 3: Spatial-Temporal distribution (every minute) of sessile microorganisms without and with conditional desorption

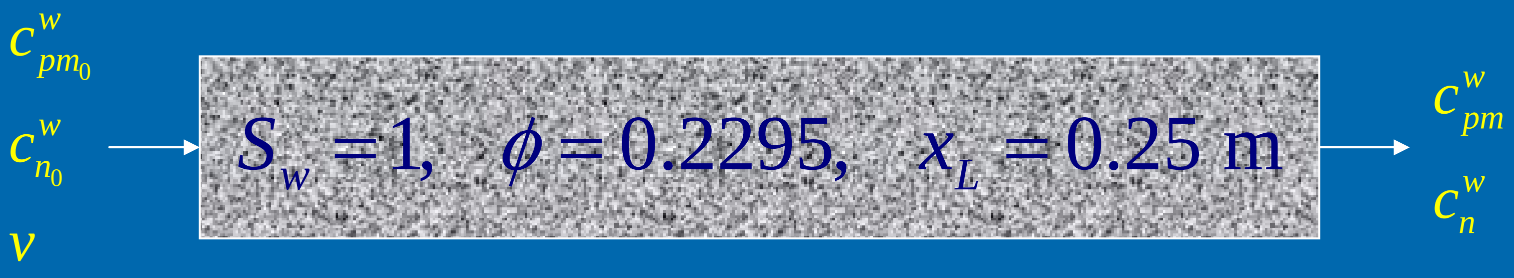
Unphysical adsorption

$\sigma \neq 0$ *for* $t \sim 0$ *at* $x = x_L$

"Clogging"

around x=0.18m for 13<t<25 minutes

Microbial/Nutrient coreflood (1)



$c^{w}_{pm_0}$

$c^{w}_{n_0}$

v

$$S_w = 1, \quad \phi = 0.2295, \quad x_L = 0.25 \text{ m}$$

c^{w}_{pm}

c^{w}_{n}

- ✓*Microbial/Nutrient solution was continuously injected*
- ✓*Sedimentation and chemotactic velocities are null.*
- ✓*There are not nutrient adsorption.*
- ✓*All others parameters will be included and used both in our model and simulations.*

Objective: To simulate a microbial/nutrient coreflood.

[5] Chang et al. "Modeling and Laboratory Investigation of Microbial Transport Phenomena in Porous Media", SPE 22845, (1991)

Microbial/Nutrient coreflood (2)

The mass local balance equation of the planktonic microorganism is:

$$\frac{\partial}{\partial t}\left(\phi c_{pm}^{w}\right)+\nabla\cdot\left(\phi c_{pm}^{w}\vec{v}-\mathbf{D}_{pm}^{w}\cdot\nabla\left(\phi c_{pm}^{w}\right)\right)=\left(\mu-k_{d}-k_{a}\right)\phi c_{pm}^{w}+k_{r}\rho_{m}\left(\sigma-\sigma_{irr}\right)$$

The mass local balance equation of the sessile microorganism is:

$$\frac{\partial}{\partial t}\left(\rho_{m}\sigma\right)=\left(\mu-k_{d}-k_{r}\right)\rho_{m}\sigma+k_{a}\phi c_{pm}^{w}+k_{r}\rho_{m}\sigma_{irr}$$

remember that the desorption term exists only if $\sigma > \sigma_{irr}$.

The total mass local balance equation of the nutrient is:

$$\frac{\partial}{\partial t}\phi c_{n}^{w}+\nabla\cdot\left(\vec{u}^{w}c_{n}^{w}-\mathbf{D}_{n}^{w}\cdot\nabla\left(\phi c_{n}^{w}\right)\right)=-\mu\left(\phi c_{pm}^{w}+\rho_{m}\sigma\right)/Y_{m/n}$$

Microbial/Nutrient coreflood (3)

Porosity	$\phi = 0.2295$
Injection rate	$u = 1\ ft/day$
Nutrients dispersion coefficient	$D_n^w = 0.0083\ ft^2/day$
Microorganisms dispersion coefficient	$D_{pm}^w = 0.0055\ ft^2/day$
Maximum specific growth rate	$\mu_{\max} = 8.4\ day^{-1}$
Monod constant	$K_{m/n} = 0.5\ lb/ft^3$
Yield coefficient	$Y_{m/n} = 0.5$
Specific decay rate	$k_d = 0.22\ day^{-1}$
Desorption rate	$k_r = 37\ day^{-1}$
Adsorption rate	$k_a = 25\ day^{-1}$
Minimum adsorbed sessile cell	$\sigma_{irr} = 0.003$
Nutrients injected concentration	$c_{n_0}^w = 2.5\ lb/ft^3$
Microorganisms injected concentration	$c_{pm_0}^w = 1.875\ lb/ft^3$

Table 4: Input data for BTCs & distributions of nutrients & microorganisms in coreflooding [5]

Microbial/Nutrient coreflood (4)

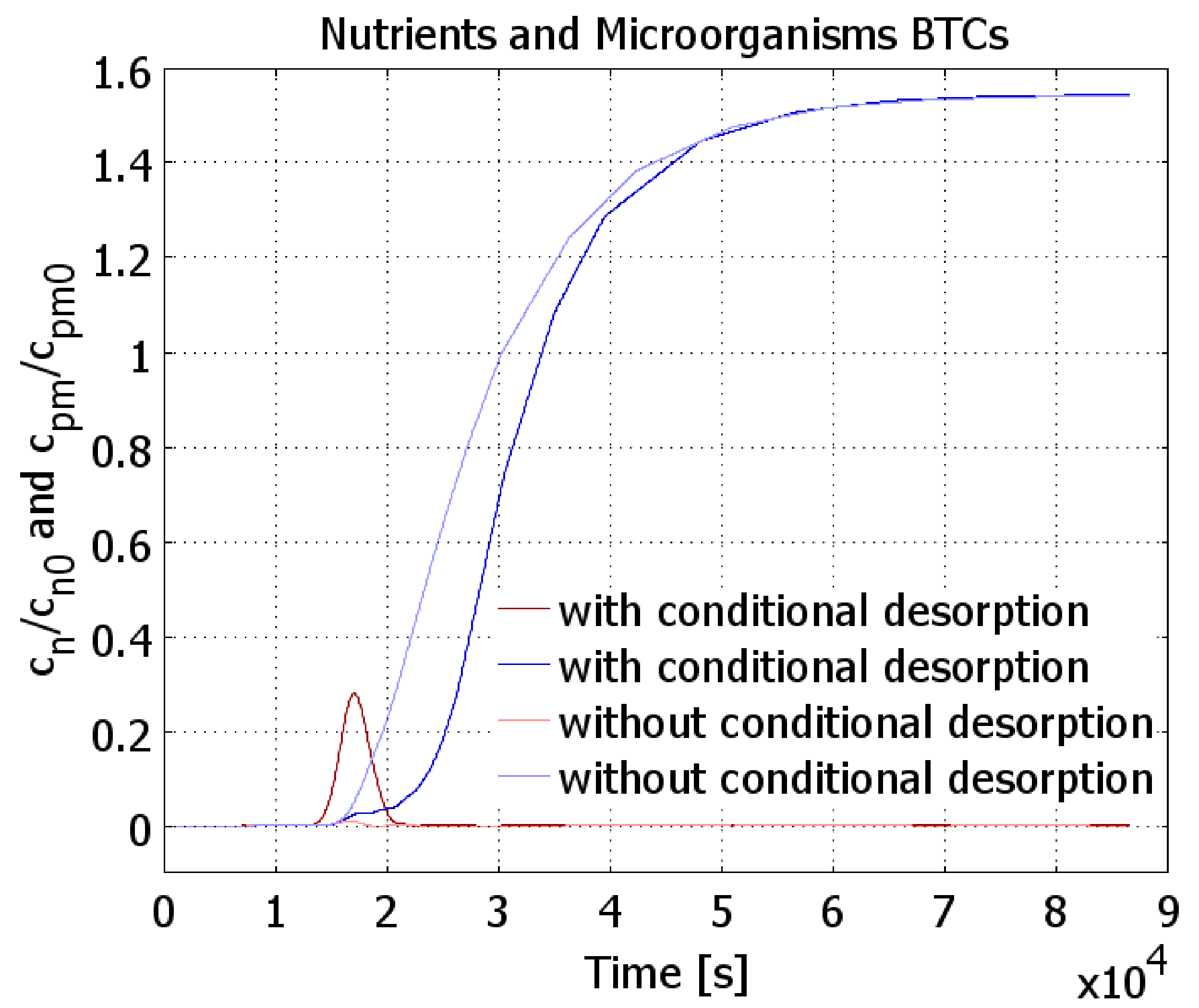


Figure 4: BTCs of nutrients (red curves) & microorganisms (blue curves) for coreflooding with and without conditional desorption

Microbial/Nutrient coreflood (5)

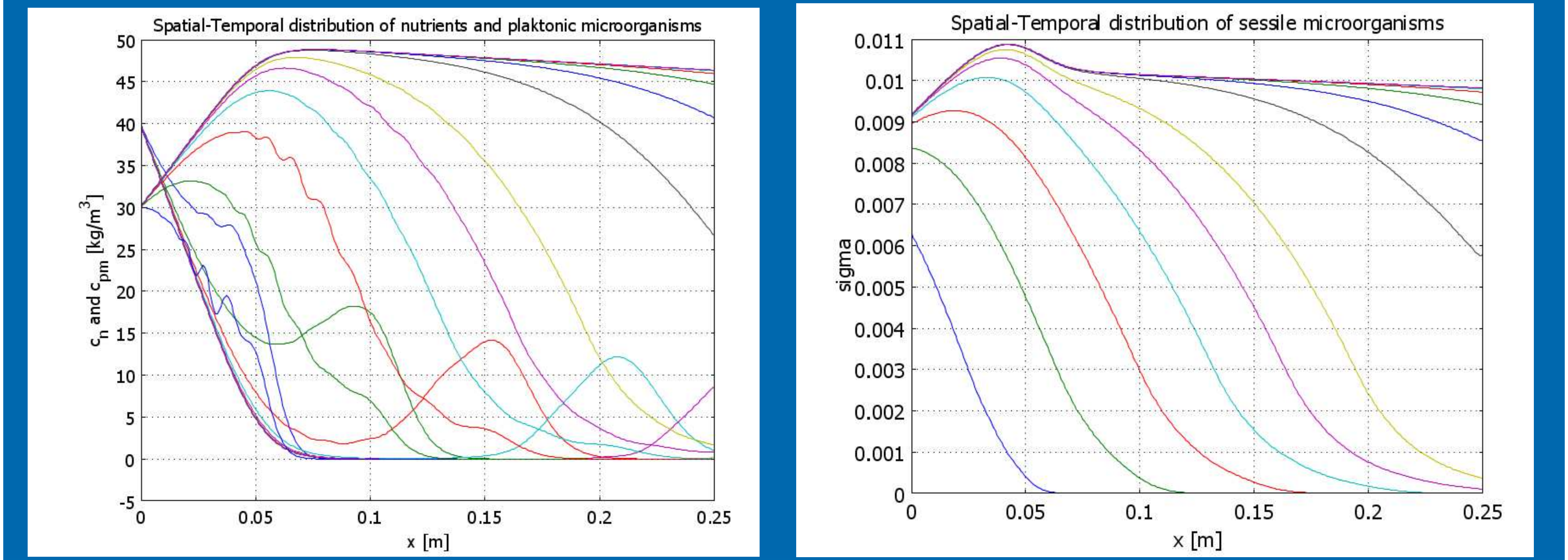
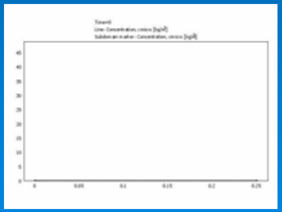
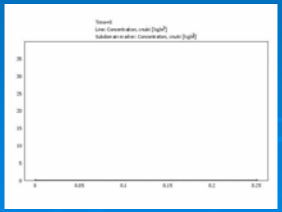
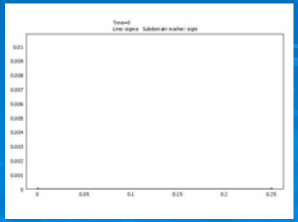


Figure 5: Spatial-Temporal distribution (every hour up to the 6th, and every 3 hours hereafter) of nutrients & planktonic microorganisms (rising from 30 kg/m³), as well as sessile microorganisms







Conclusions

We derive a very complete model, we implement a numerical model into COMSOL Multiphysics environment, and we perform simulations which can be used to analyze some phenomena involved in transport of microorganisms and nutrients through porous media.

We point out the complementary role of the spatial-temporal distribution of components relative to the BTCs, because the BTCs alone do not render complete information about the behavior of both fluent and adsorbed components.

Perspectives

A first successful step in modeling the fate of microorganisms through porous media has been done.

In order to obtain a more complete and sound model, it is required to couple the present model with a flow model like that which was presented by M.A. Diaz-Viera et. al., in this same session of the conference.

Furthermore, some aspects as chemotactic of microorganisms and adsorption of nutrients, will be simulated soon.

References

[1] Allen et al. "Numerical modeling in science and engineering", John Wiley & Sons., USA, (1988)

[2] COMSOL Multiphysics, Earth Science Module, User's Guide Version 3.3, 37, COMSOL LAB (2006)

[3] Tan et al. "Transport of bacteria in an aquifer sand: Experiments and model simulations", Water Resources Research, 30 (12), 3243-3252, (1994)

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[5] Chang et al. "Modeling and Laboratory Investigation of Microbial Transport Phenomena in Porous Media", SPE 22845, (1991)

Thanks for your attention!

¡Gracias por su atención!