Universidad de los Andes

Presented at the 2011 COMSOL Conference in Boston

Model of a Heavy Metal Adsorption System Using the S-Layer of *Bacillus sphaericus*

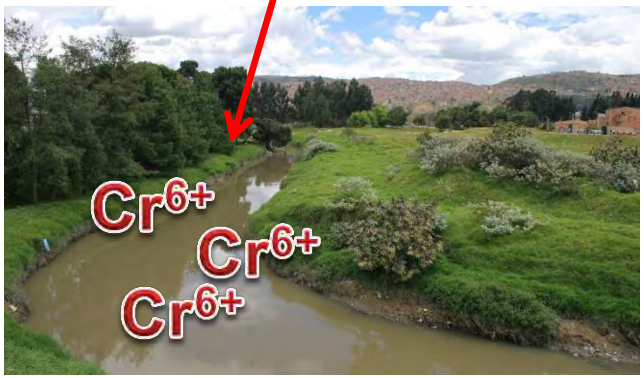
Juan Pablo Orjuela

Urban and Regional Sustainability Group
Universidad de los Andes
Bogota - Colombia

Universidad de los Andes

Heavy metals and water

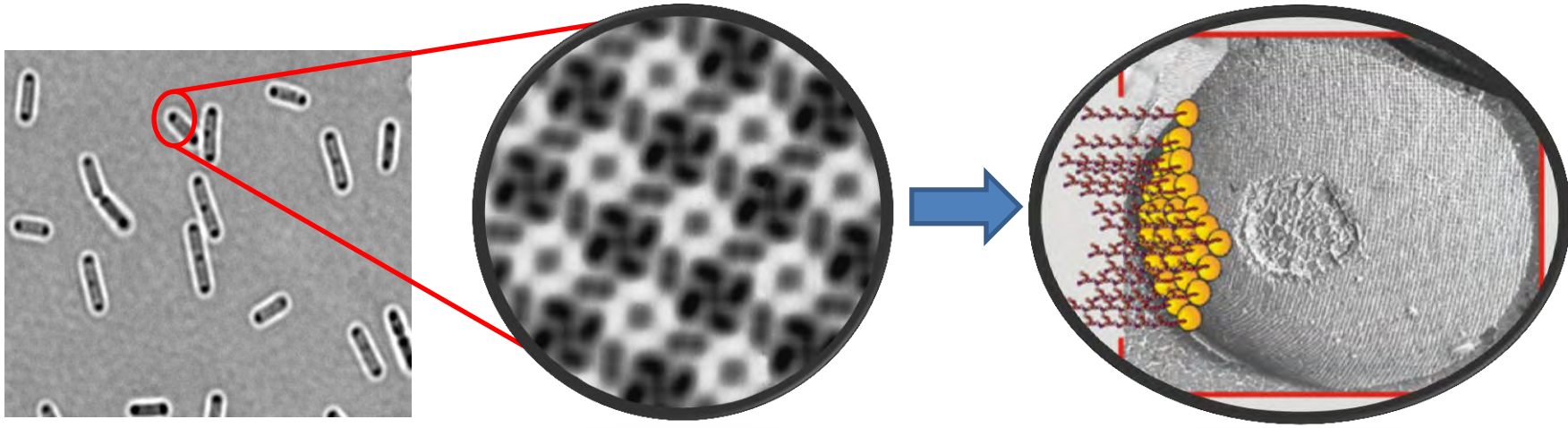
+ Cr =



Universidad de los Andes

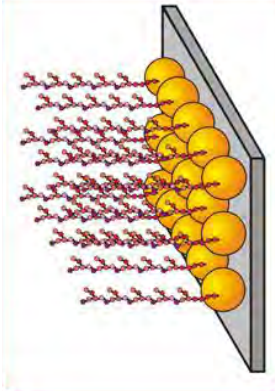
Cr^{6+} Cr^{6+} Cr^{6+}
Cr^{6+} Cr^{6+} Cr^{6+} Cr^{6+}

Bacillus sphaericus



Universidad de los Andes

Tunjuelito meets *Ba*



Universidad de los Andes

Let's model this!

$$\varepsilon_e \frac{\partial C_i}{\partial t} + \rho_p (1 - \varepsilon_e) \frac{\partial \bar{q}_i}{\partial x} + \varepsilon_e \frac{\partial (u.C_i)}{\partial z} = \varepsilon_e (E + D_m) \frac{\partial^2 C_i}{\partial z^2}$$

$$\rho_p \, (1-\varepsilon_e) \frac{\partial \bar{q}_i}{\partial t} = K_m . a_p \, [C_i - C_i{}^*]$$

- Langmuir's Isotherm

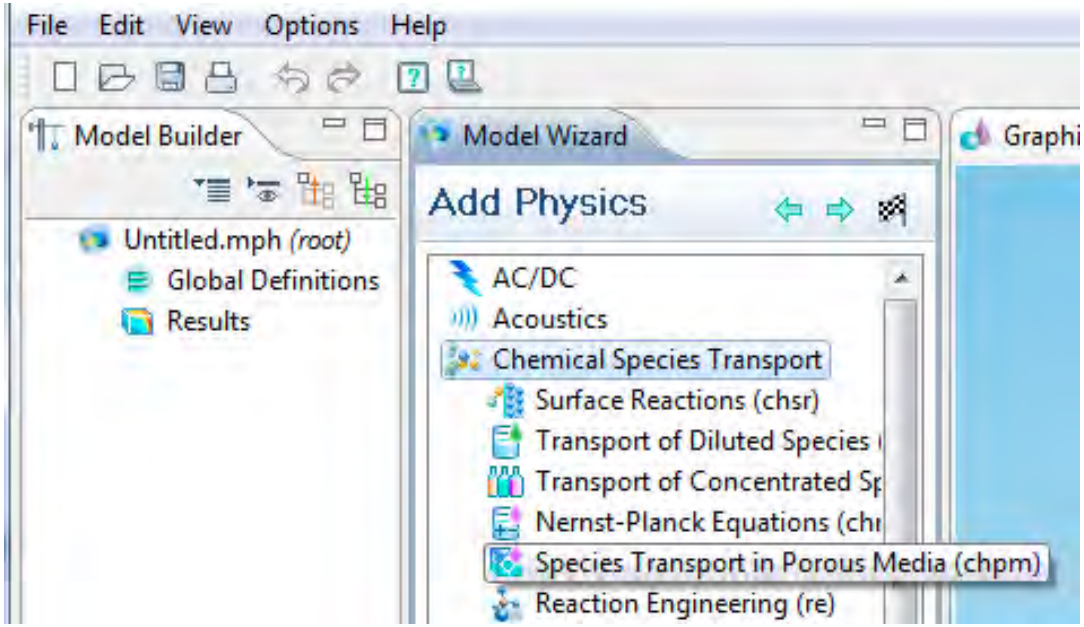
$$q_i = \frac{Q C_i^*}{k + C_i^*}$$

Universidad de los Andes

Use of COMSOL Multiphysics

- 2D
- Mass transfer module
- Chemical Species Transport / chpm

$$\delta \frac{\partial c_i}{\partial t} + \nabla \cdot (-D_i \nabla c_i) = R_i - \mathbf{u} \nabla \cdot c_i$$



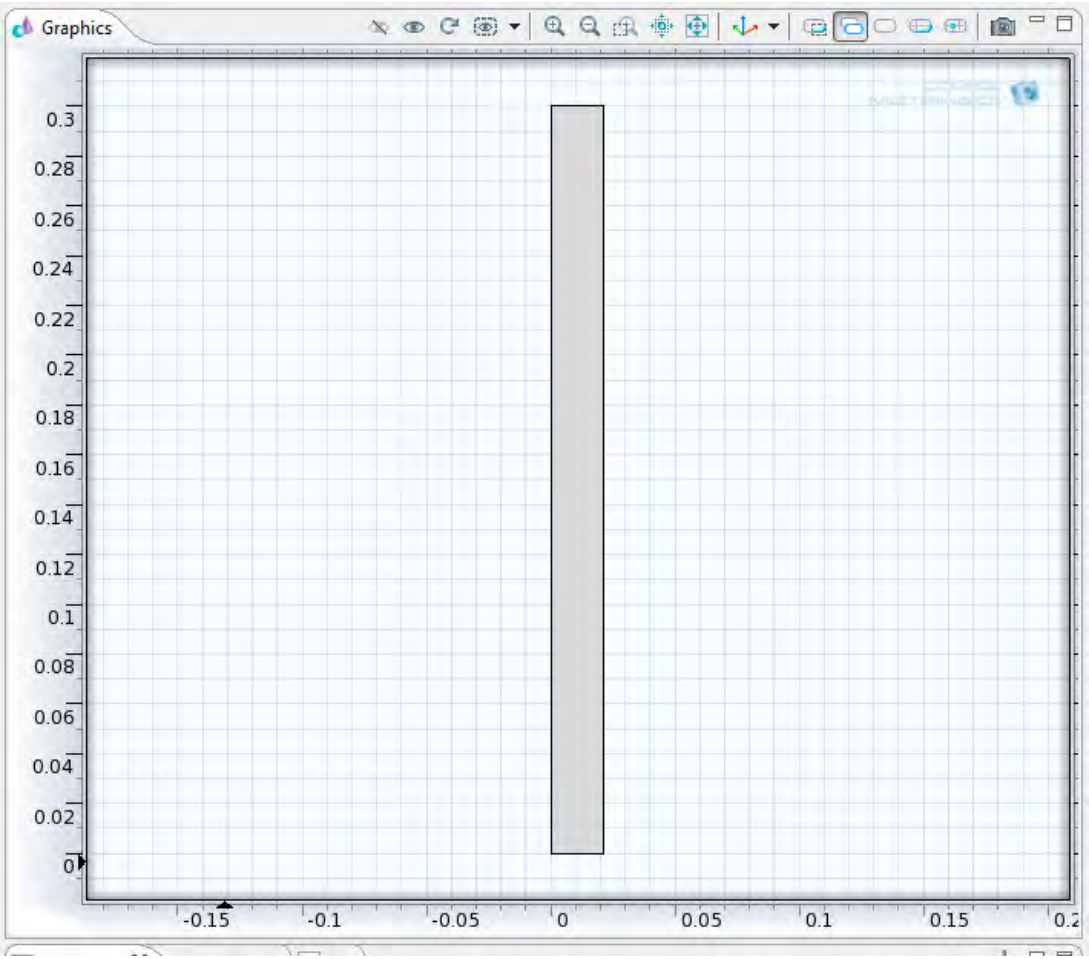
Universidad de los Andes

Global parameters

- Experimental:
  - Langmuir
  - Time for saturation
  - Density
  - Porosity
  - Initial concentrations
- Literature:
  - Dm
  - E
  - Km

Universidad de los Andes

Geometry



Universidad de los Andes

Species transport in porous media

Equation

Show equation assuming:

Study 1, Time Dependent

$$P_{1,i}\frac{\partial c_i}{\partial t} + P_{2,i} + \nabla \cdot \boldsymbol{\Gamma}_i + \mathbf{u} \cdot \nabla c_i = R_i + S_i$$

$$P_{1,i} = (\epsilon + \rho_b k_{p,i})$$

$$P_{2,i} = (c_i - c_{p,i}\rho_p)\frac{\partial \epsilon}{\partial t}, \quad \rho_p = \frac{\rho_b}{(1-\epsilon)}$$

$$\mathbf{N}_i = \boldsymbol{\Gamma}_i + \mathbf{u}c_i = -(D_{D,i} + D_{e,i})\nabla c_i + \mathbf{u}c_i$$

Model Inputs

Coordinate System Selection

Porous Media

Porosity:

ϵ eps 1

Bulk density:

ρ_b rho*(1-eps) kg/m^3

Adsorption

Species c:

Langmuir

$$c_{p,i} = \frac{k_{L,i}c_{p,max,i}c_i}{1 + k_{L,i}c_i}, \quad k_{p,i} = \frac{\partial c_{p,i}}{\partial c_i} = \frac{k_{L,i}c_{p,max,i}}{(1 + k_{L,i}c_i)}$$

Langmuir constant:

$k_{L,c}$ b m^3/mol

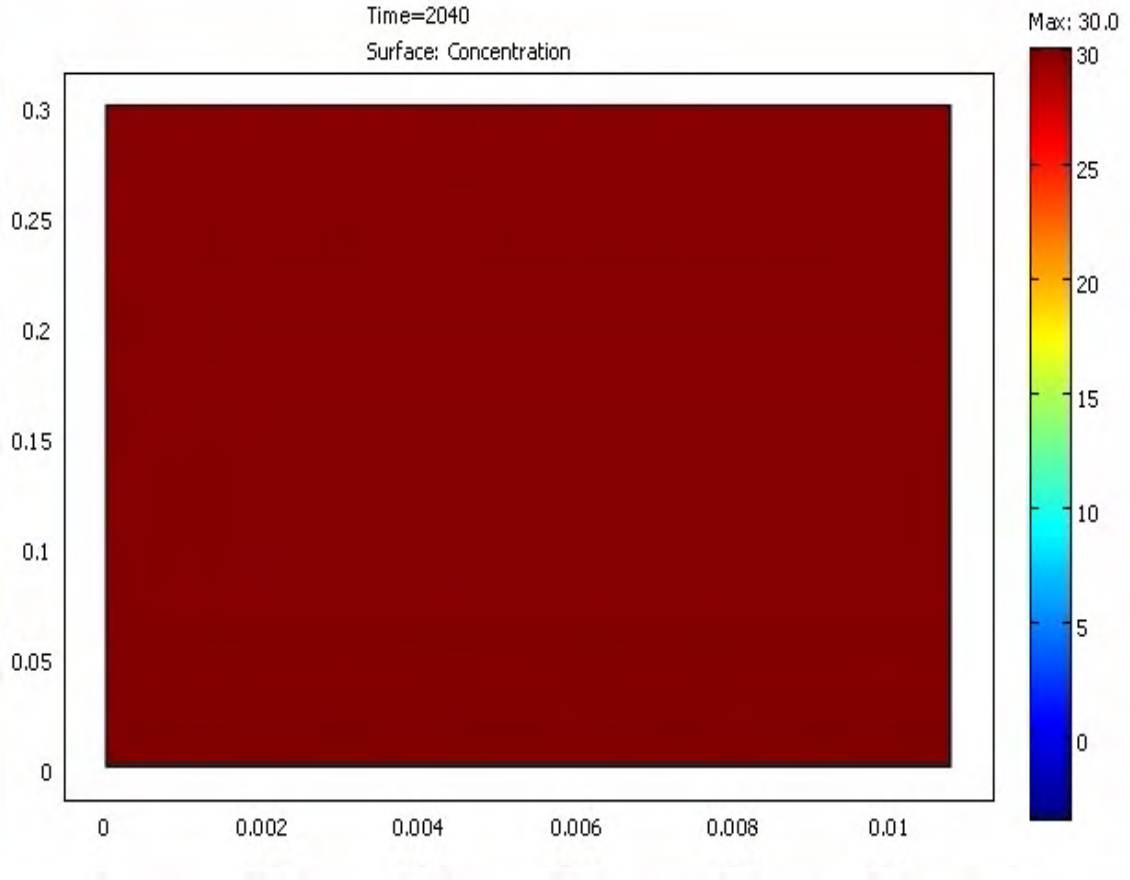
Adsorption maximum:

$c_{p,max,c}$ Qo*S mol/kg

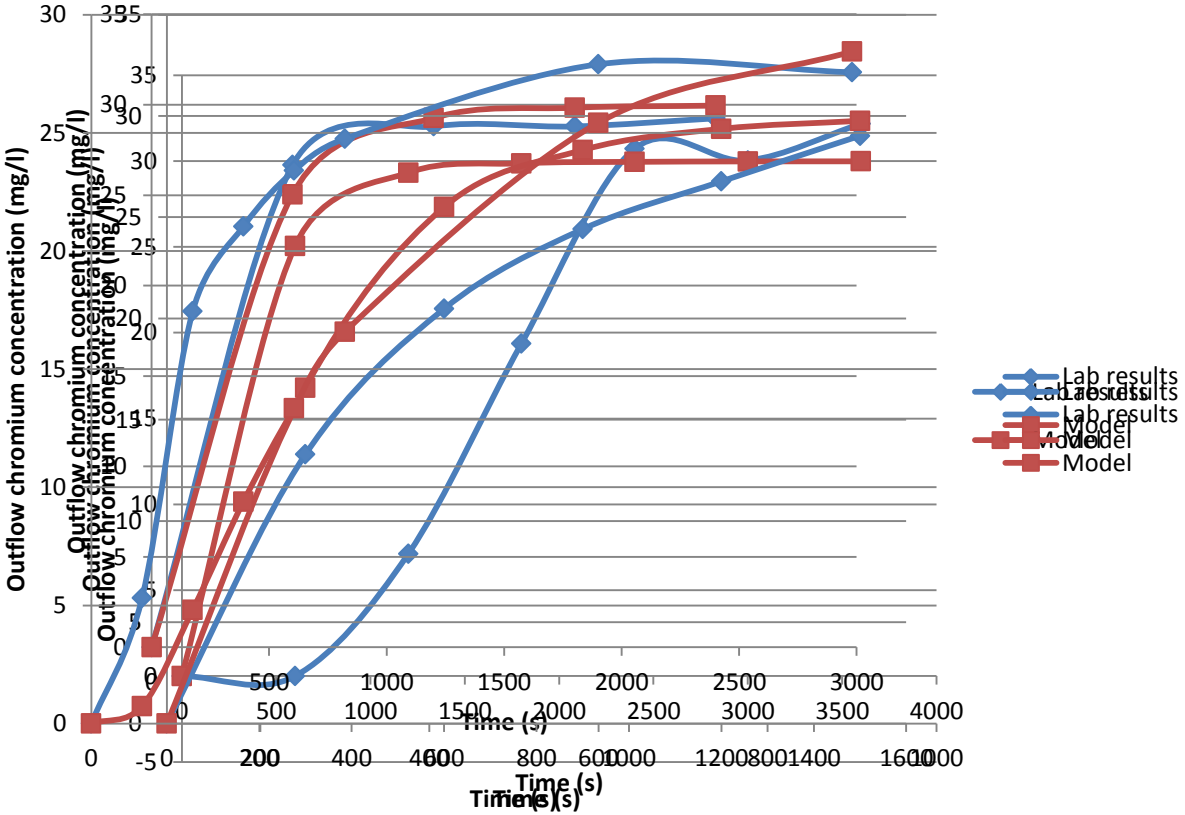
Dispersion

Universidad de los Andes

Results

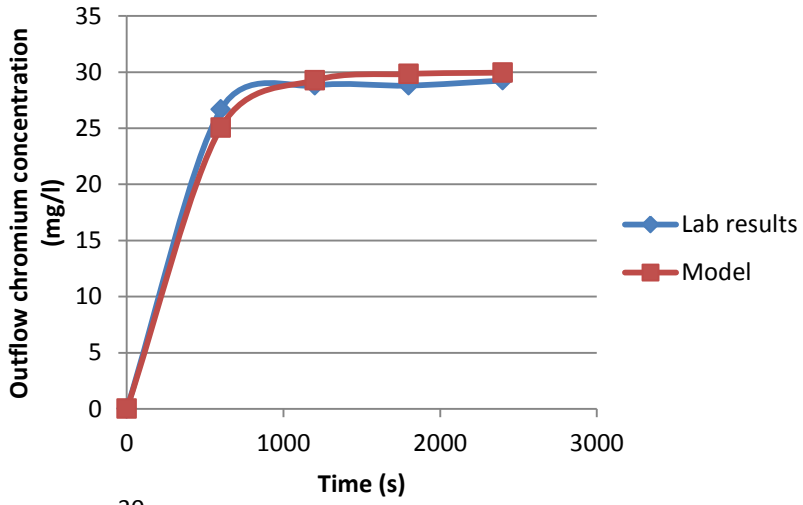


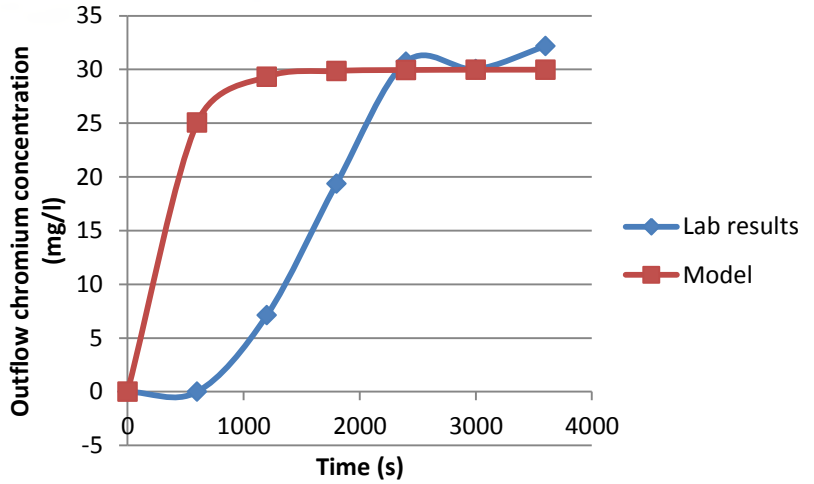
Results II

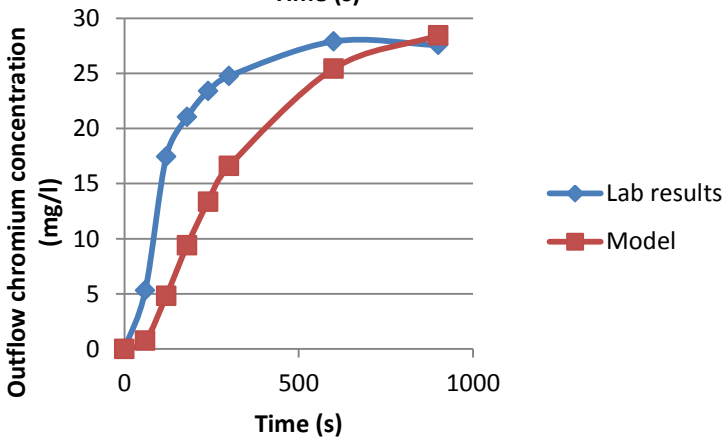

Outflow chromium concentration (mg/l)
Time (s)
Lab results
Model

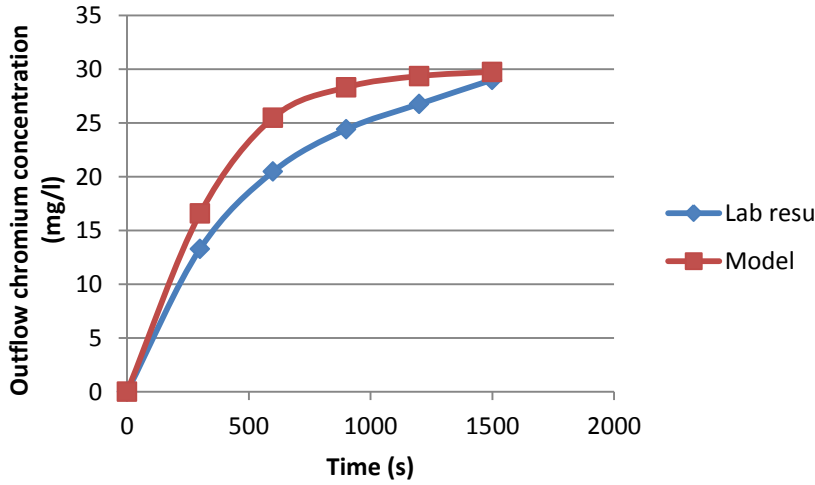
Universidad de los Andes

Results II









Universidad de los Andes

Conclusions

- The model shows some really good preliminary results
- 1-D analysis is a good option
- Particle size has a greater effect than inflow speed
- Relationship between surface area and diffusivity coefficient ?
- Scale-up?

Universidad de los Andes

Acknowledgements

- Civil and Environmental Engineering Department
- Urban and Regional Sustainability Group
- Chemical Engineering Department
- Biology Department
- Nathalia Flórez
- Andrea García
- Andrés Gonzalez

Universidad de los Andes

THANK YOU!

Juan Pablo Orjuela
jua-orju@uniandes.edu.co