Interpore 2019 - 8 May 2019 - Valencia

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Modeling solute transport in segregated porous media:

Sensitivity-driven calibration of a new double continuum model

Giulia Ceriotti[1], Anna Russian[1], Diogo Bolster[2] & Giovanni Porta[1]

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Transport modeling in porous media:

Lagrangian and Eulerian approaches (e.g., Russian et al., 2016; Bijeljic et al, 2013; Dentz and Castro, 2009; Porta et al. 2015; de Anna et al., 2017; ; Berkowitz et al., 2002; Le Borgne et al., 2008; Alhashmi et al., 2016; Tecklenburg et al., 2016; Haggerty and Gorelick, 1995; Carrera et al., 1998; Berkowitz and Scher, 2009; Berkowitz and Scher, 1997; Neuman and Tartakovsky, 2009; Kelly et al., 2017;Wirner et al., 2014; Puyguiraud et al. 2019; Davit et al., 2012)

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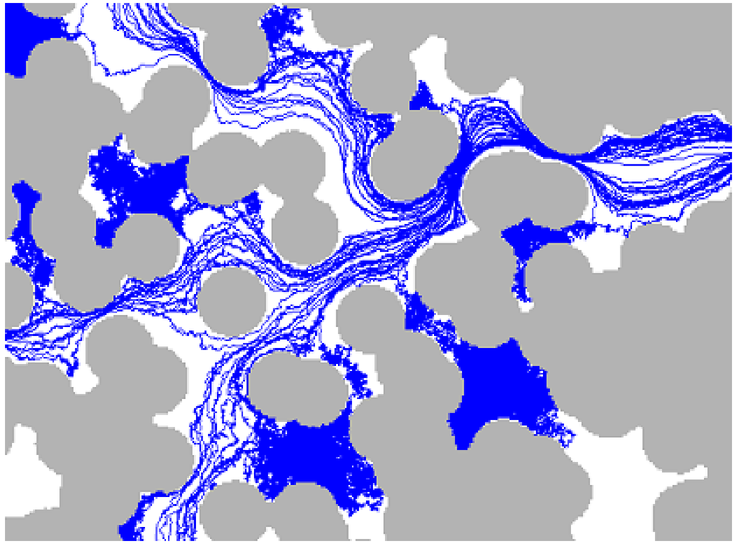
The challenge in segregated porous media:

(Kapoor et al., 1997; Raje and Kapoor, 2000)

ϕ=0.23

Average velocity 6μm/s

t = 20h



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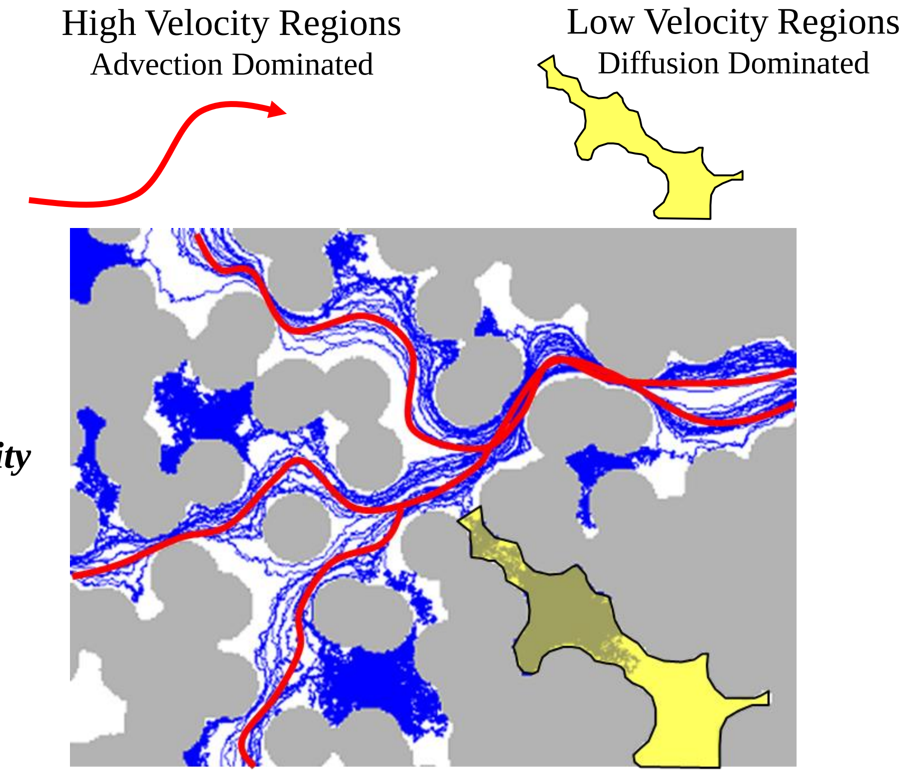

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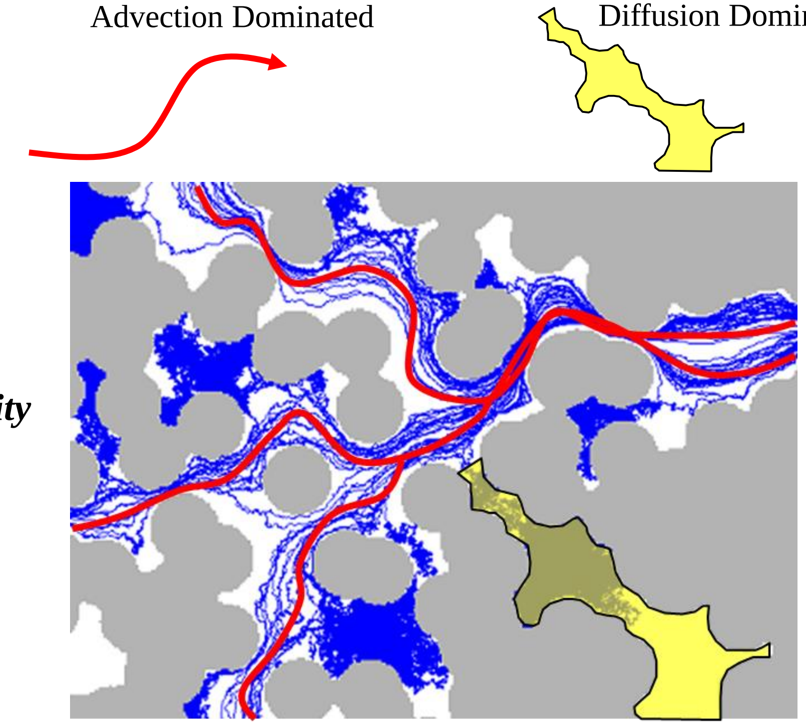
High Velocity Regions
Advection Dominated

Low Velocity Regions
Diffusion Dominated



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(Wirner et al.,2014)

We focus on the Eulerian Approach

For example Double or Multi-Rate Mass Transfer Model:

- Geometry information
- Non-local terms, computationally intense

(Davit et al., 2012, Porta et al., 2016)

Transport Modeling in Segregated Porous media

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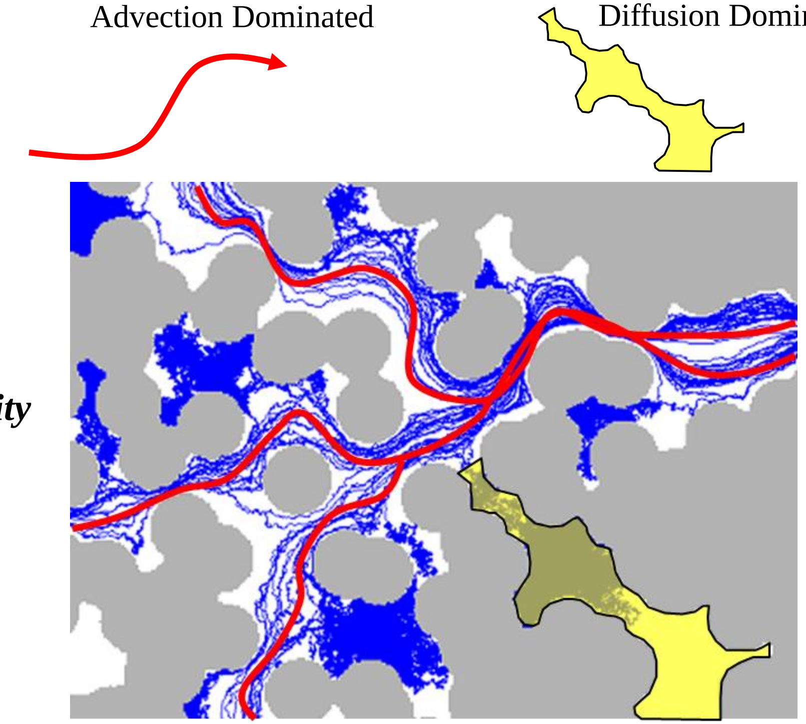

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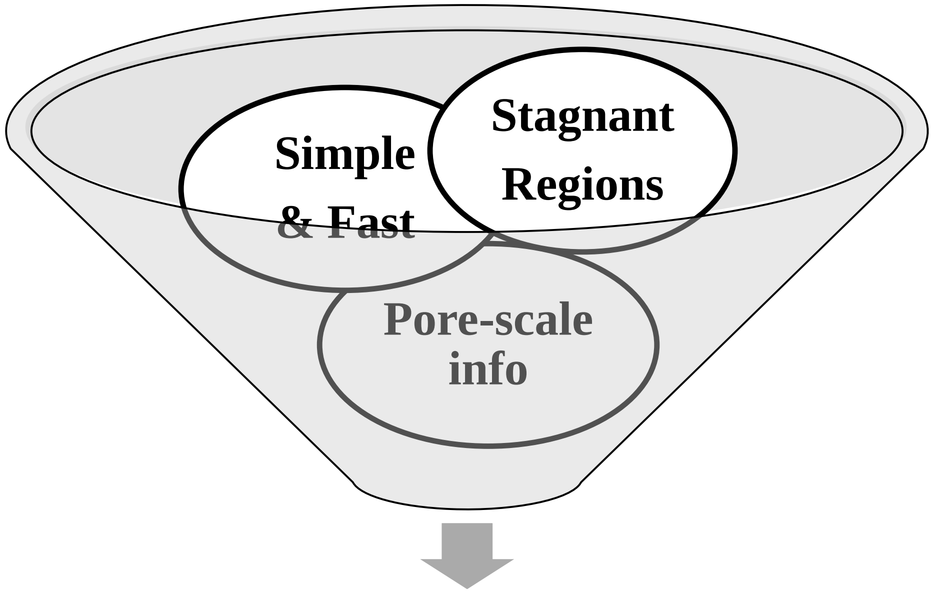
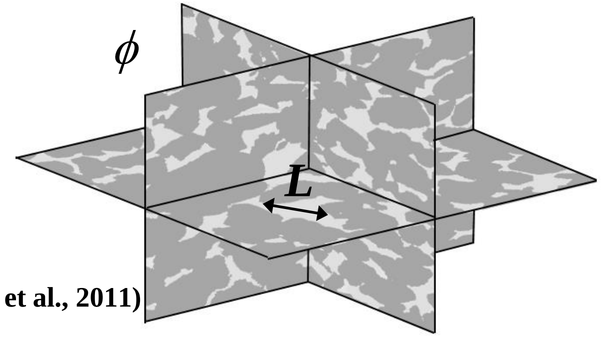
Our Aim:



1-D Continuum Model

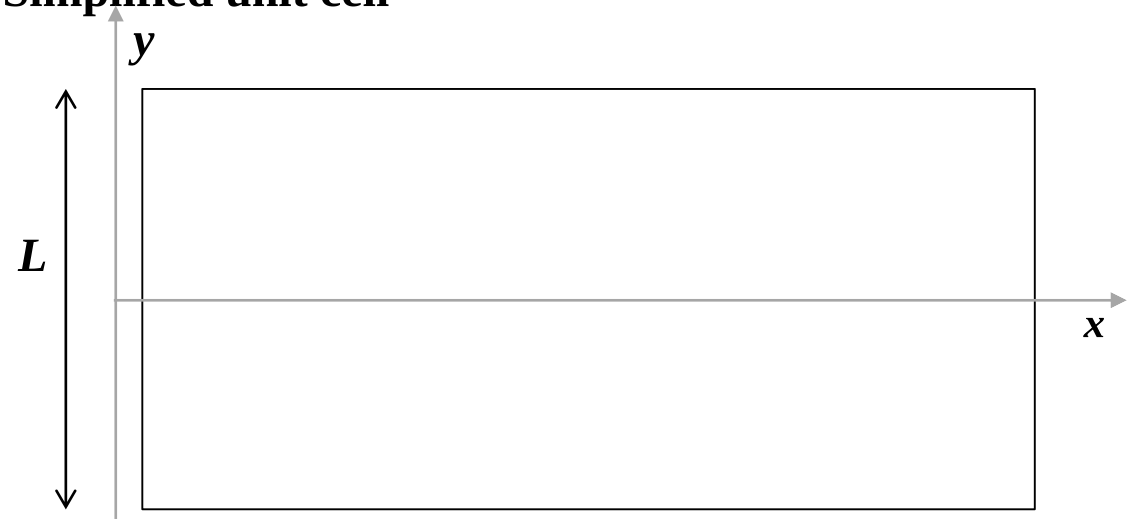
The Continuum Model

Real porous medium (L, ϕ)



(Bijeljic et al., 2011)

Simplified unit cell



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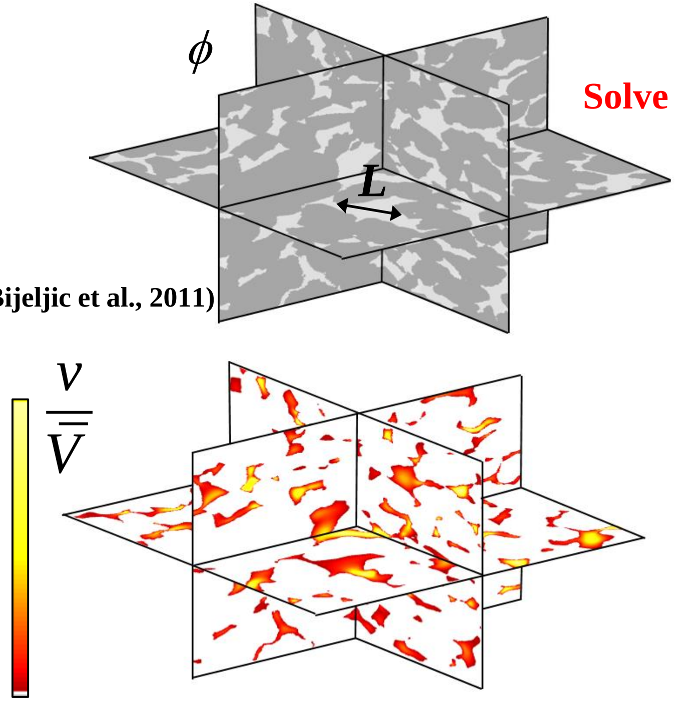

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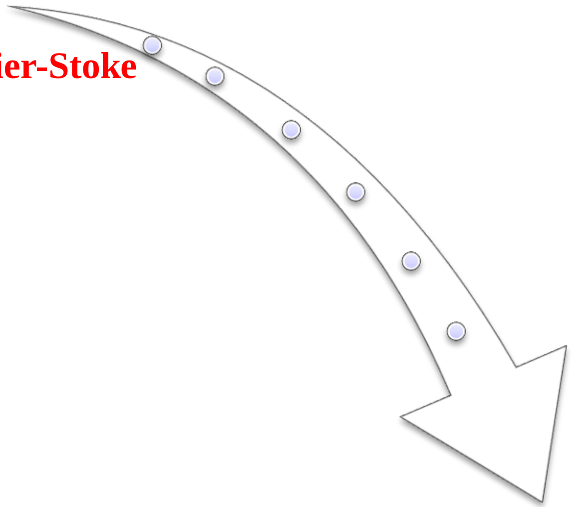

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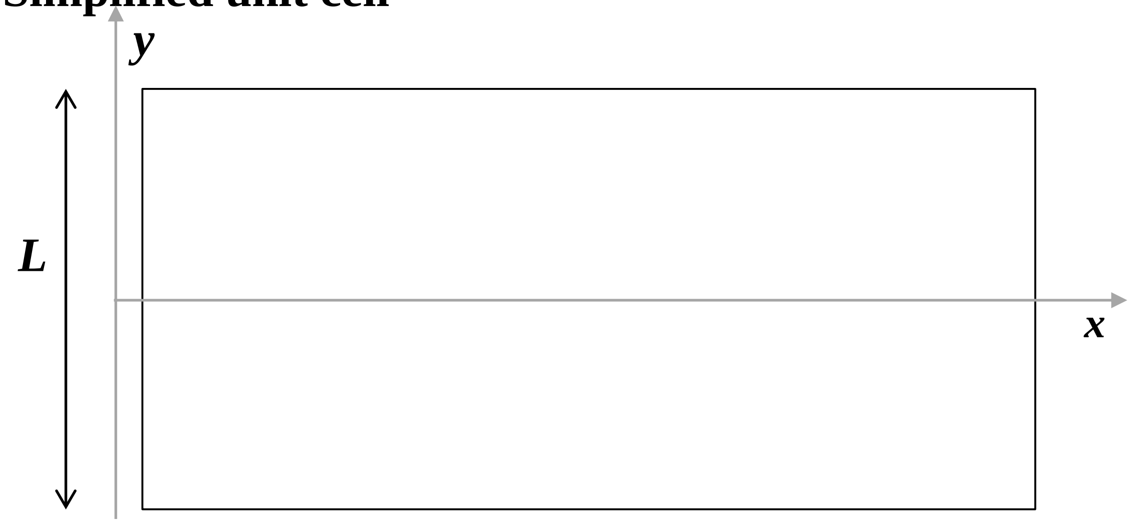

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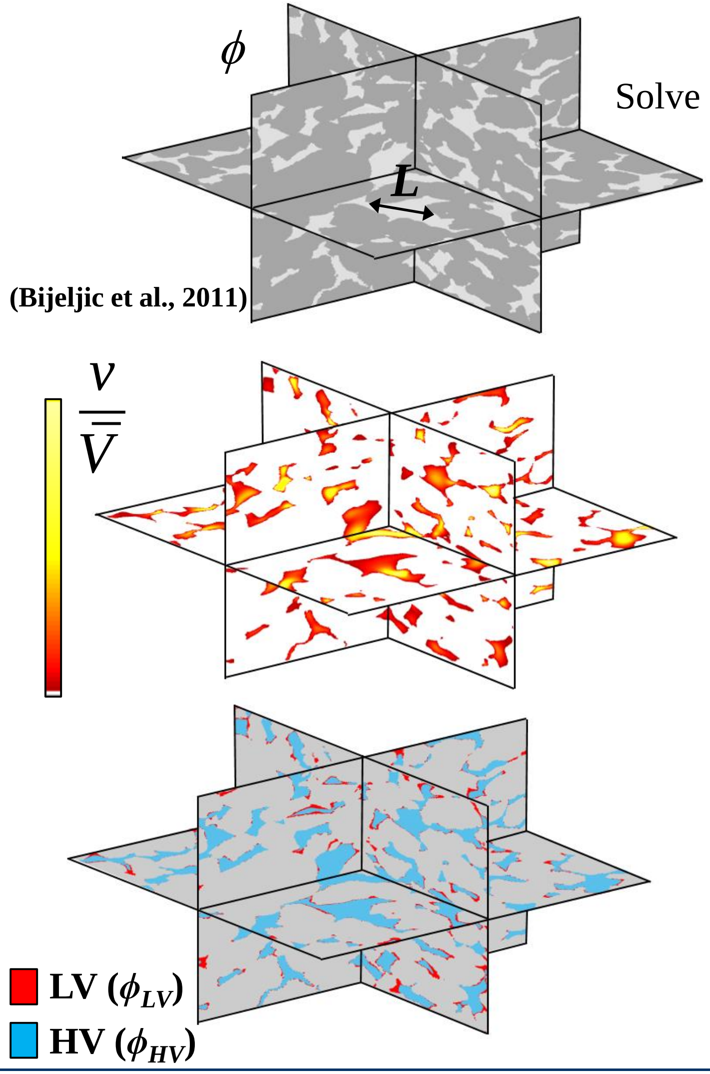
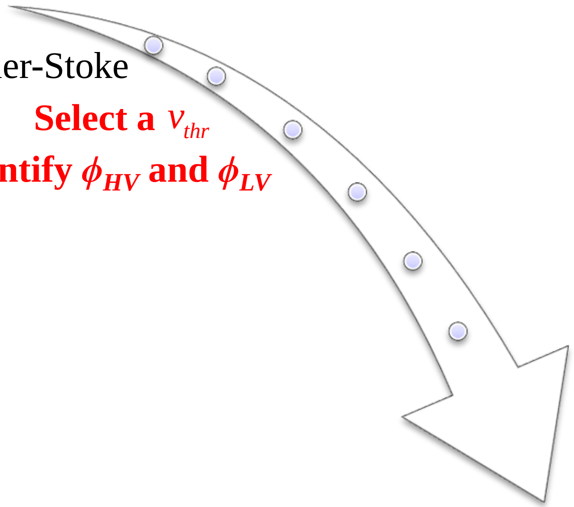


(Bijeljic et al., 2011)

Solve Navier-Stoke

Select a v_{thr}

Identify ϕ_{HV} and ϕ_{LV}



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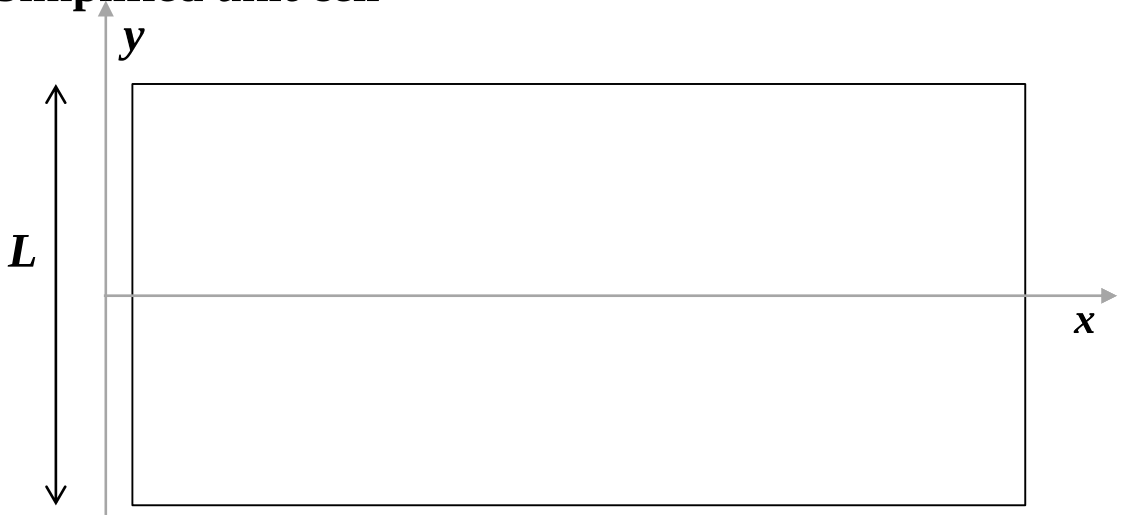

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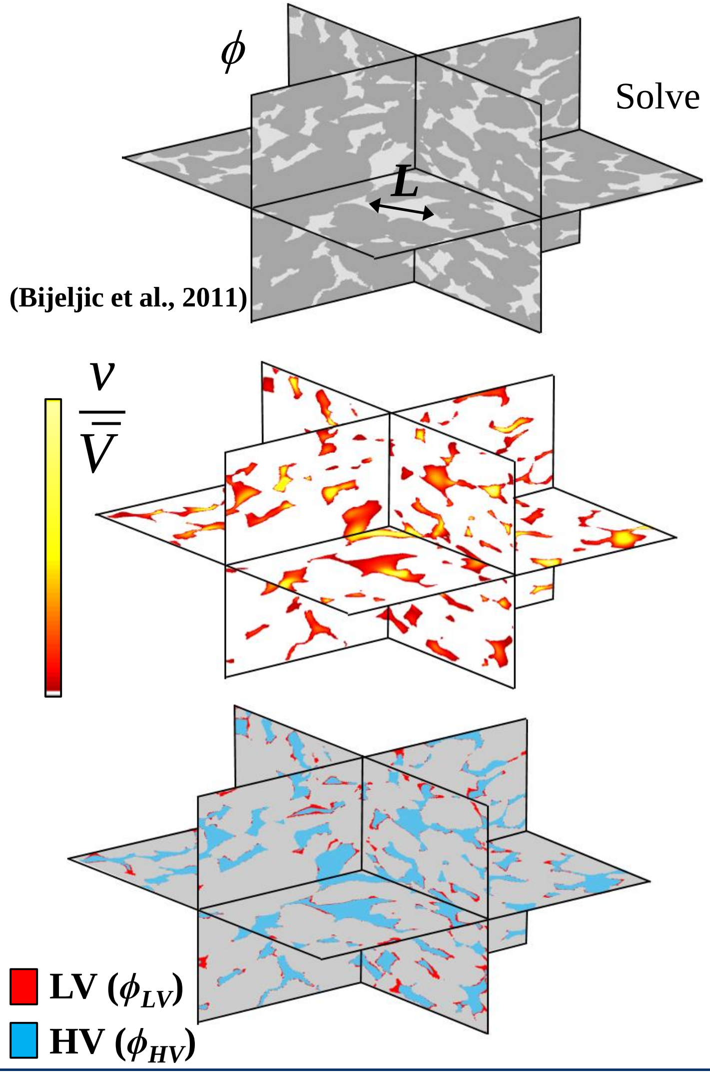

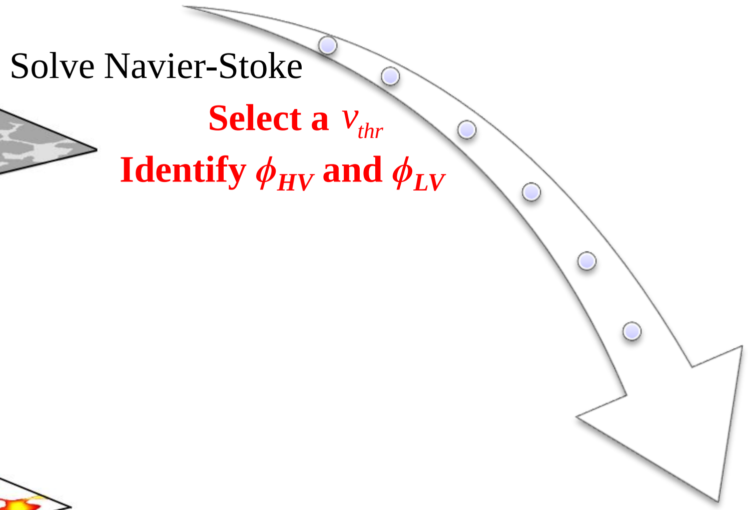

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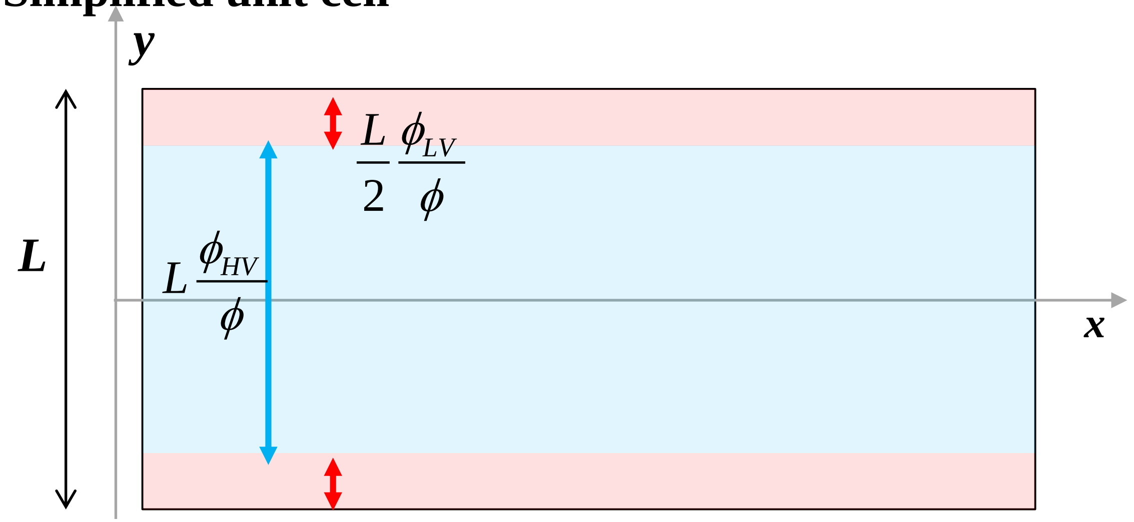

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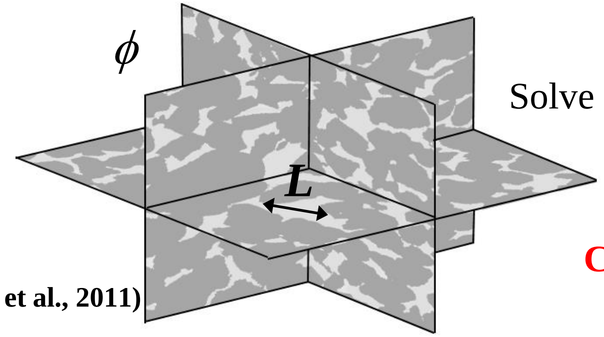

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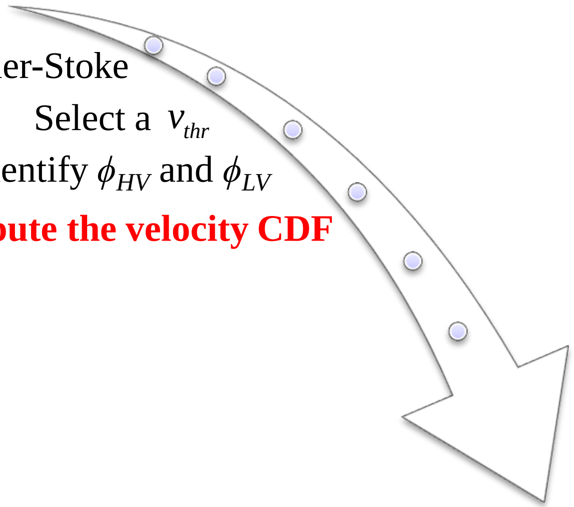

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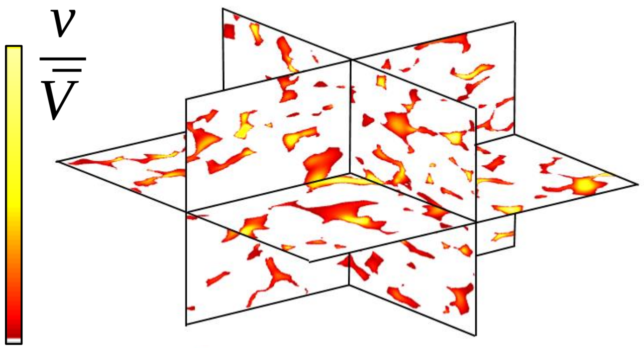
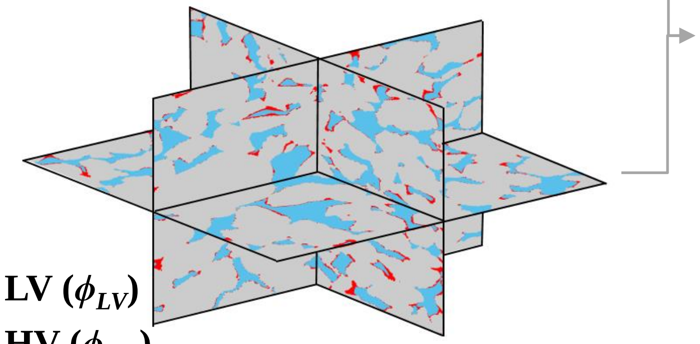
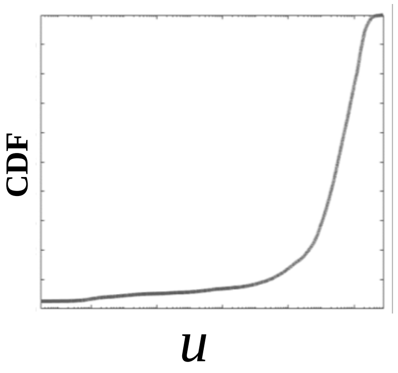




LV (ϕ_{LV})

HV (ϕ_{HV})



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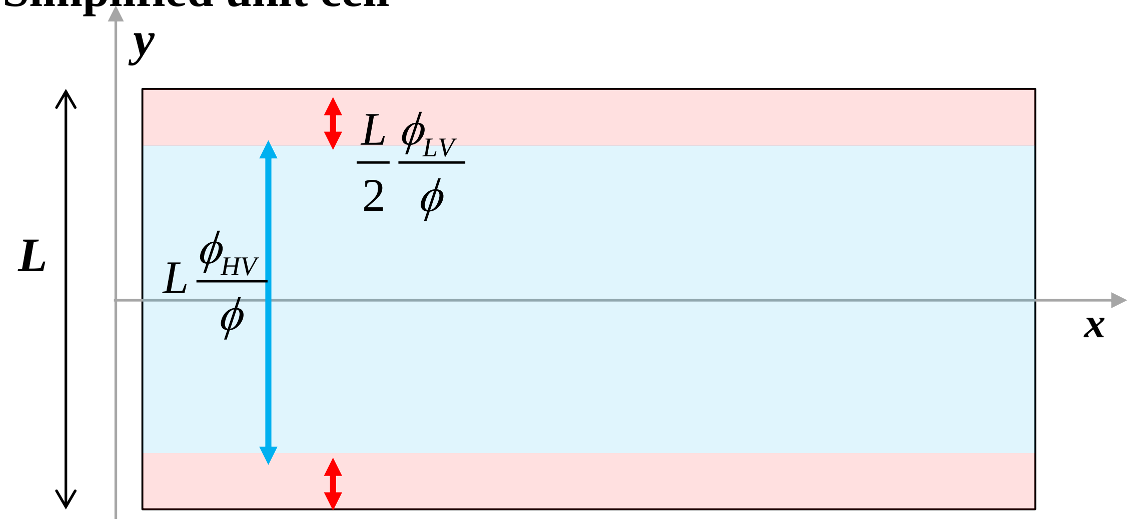

The Continuum Model

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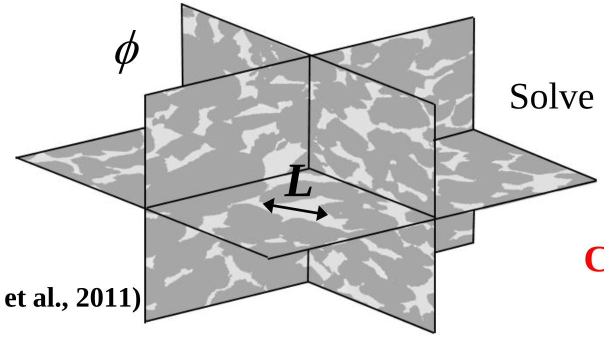

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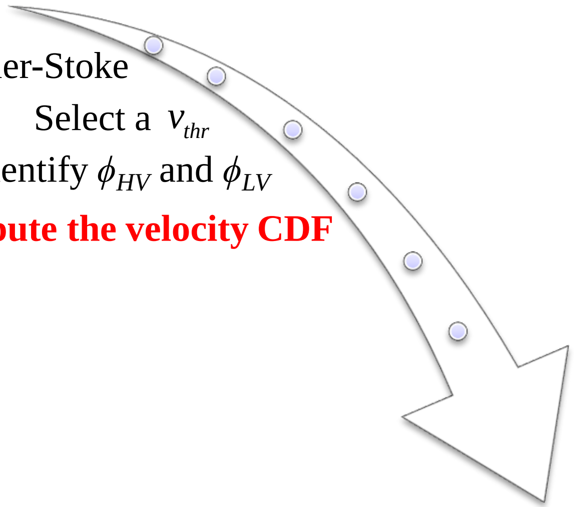

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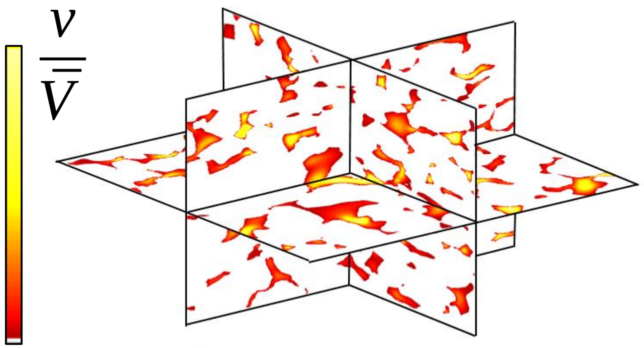

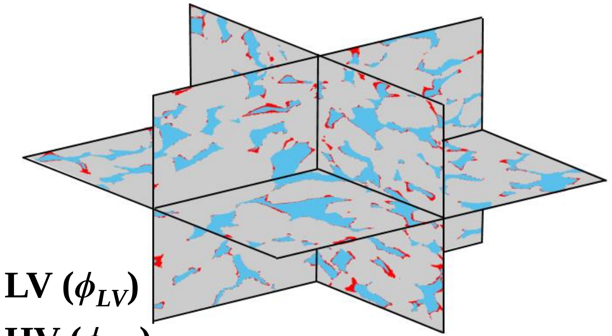

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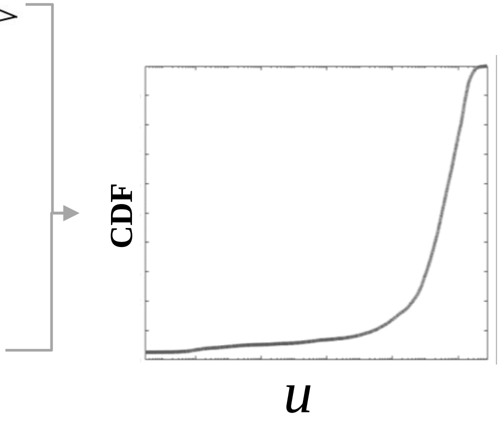

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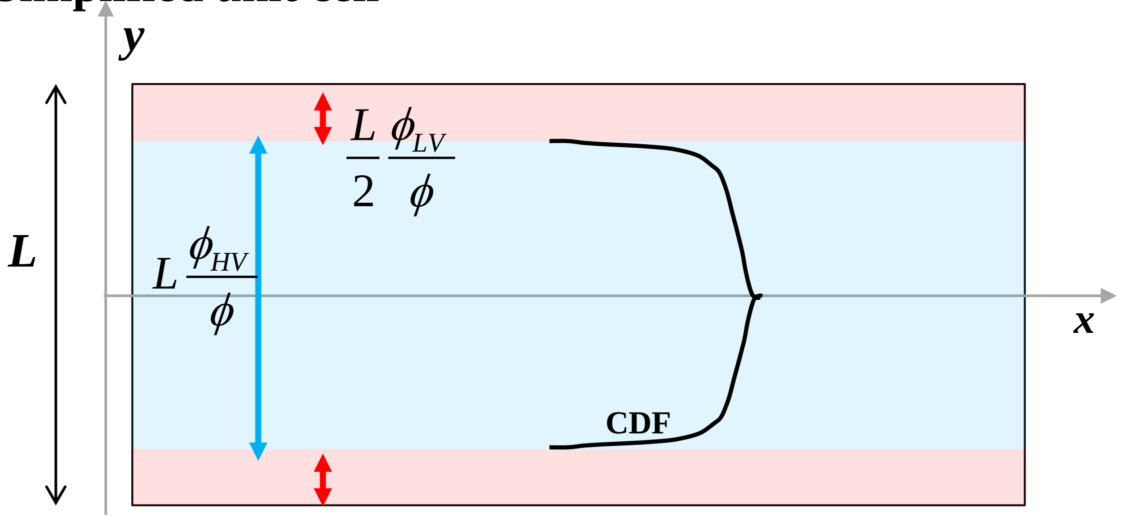

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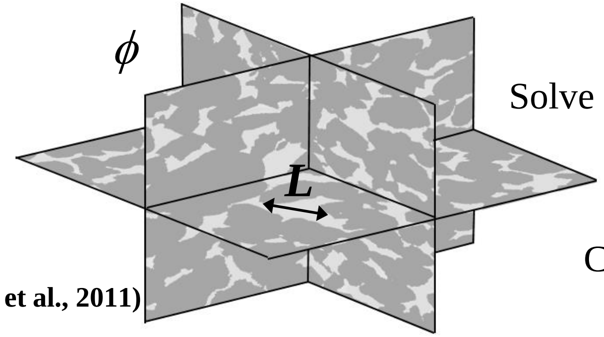

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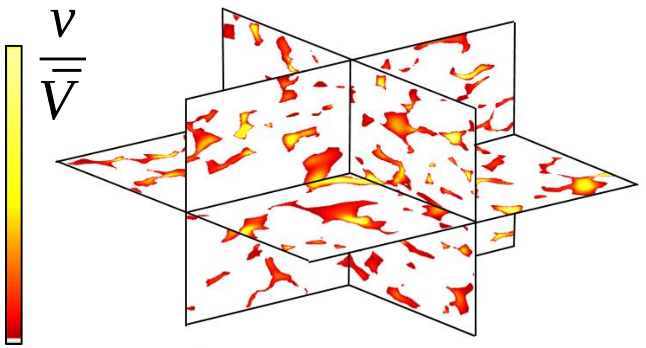

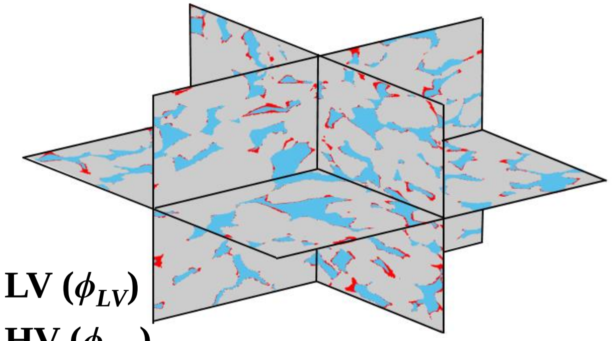

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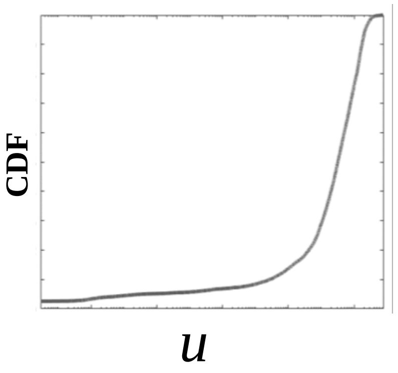


Define the unit cell equations

Transport in the unit cell

$$\begin{cases} \dfrac{\partial c_M}{\partial t} + u\dfrac{\partial c_M}{\partial x} = \dfrac{1}{Pe}\dfrac{1}{\tau_M}\dfrac{\partial^2 c_M}{\partial x^2} + \dfrac{1}{Pe}\dfrac{\partial^2 c_M}{\partial y^2} & |y| < l/(2L) \\ \dfrac{\partial c_I}{\partial t} = \dfrac{1}{Pe}\dfrac{1}{\tau_{IM}}\dfrac{\partial^2 c_I}{\partial x^2} + \dfrac{R_D}{Pe}\dfrac{\partial^2 c_I}{\partial y^2} & |y| > l/(2L) \end{cases}$$

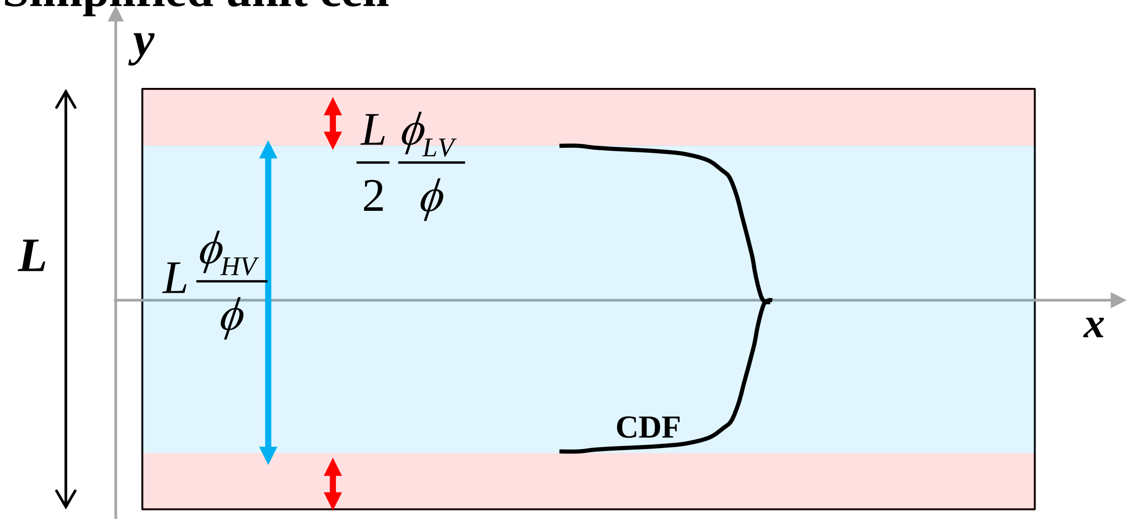
$$R_D = \frac{t_d}{t_e}$$

Boundary Conditions

$$c_M = c_I \quad \text{and} \quad \frac{\partial c_M}{\partial y} = R_D\frac{\partial c_I}{\partial y} \qquad |y| = l/(2L)$$

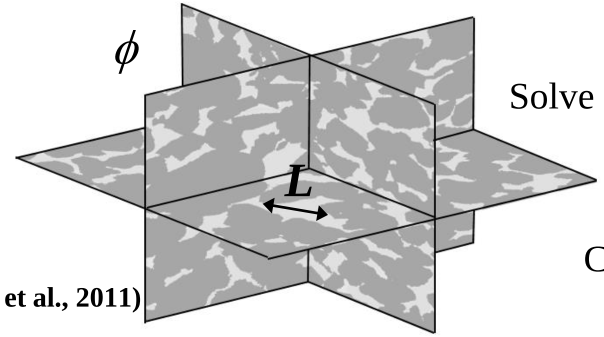
$$\frac{\partial c_I}{\partial y} = 0 \qquad |y| = 1/2$$

Simplified unit cell



The Continuum Model

Real porous medium (L, ϕ)



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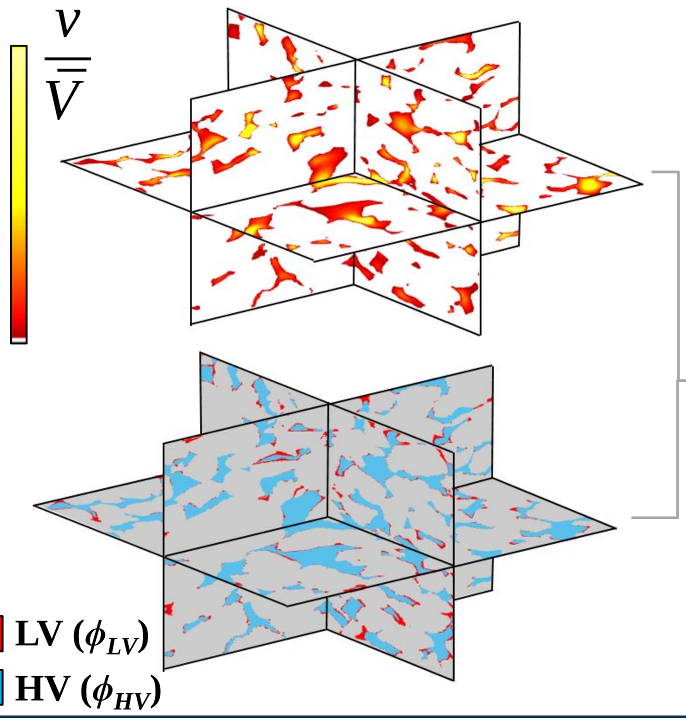

LV (ϕ_{LV})

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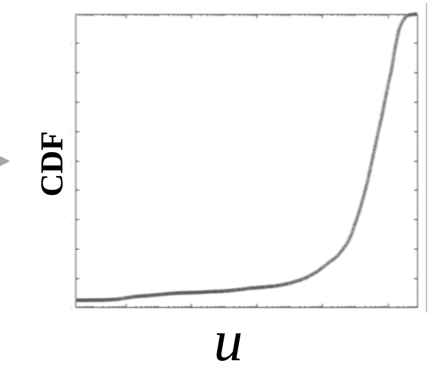


Define the unit cell equations

Average along y

Averaged equations along the y-direction

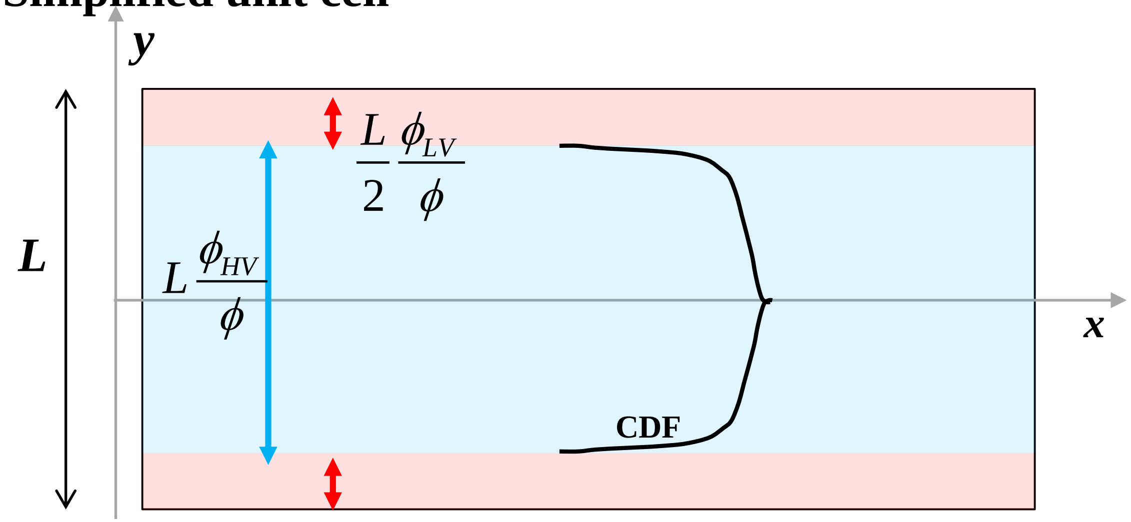
$$\begin{cases} \frac{\partial C_M}{\partial t} + \frac{\partial C_M}{\partial x} + \frac{\partial}{\partial x}\left[d_{H1}\frac{\partial C_M}{\partial x} + d_{H2}\Delta C_{MI} \right] = \frac{1}{Pe}\frac{1}{\tau_M}\frac{\partial^2 C_M}{\partial x^2} + \frac{\phi}{Pe\phi_{HV}}\left(e_1\frac{\partial C_M}{\partial x} + e_2\Delta C_{MI} \right) \\ \frac{\partial C_I}{\partial t} = \frac{1}{\tau_{IM}}\frac{1}{Pe}\frac{\partial^2 C_I}{\partial x^2} - \frac{\phi}{\phi_{LV} Pe}\left(e_1\frac{\partial C_M}{\partial x} + e_2\Delta C_{MI} \right) \end{cases}$$

Closure Variables

$e_1 \quad e_2 \longrightarrow f(RD)$

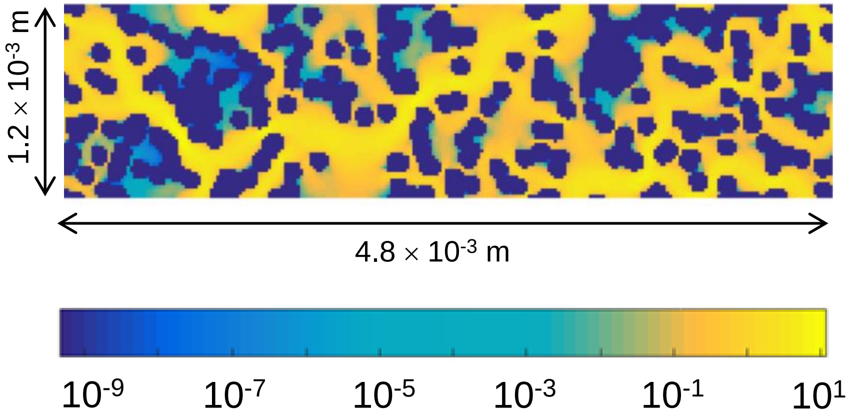
$d_{H1} \quad d_{H2}$

Simplified unit cell



Model calibration and validation

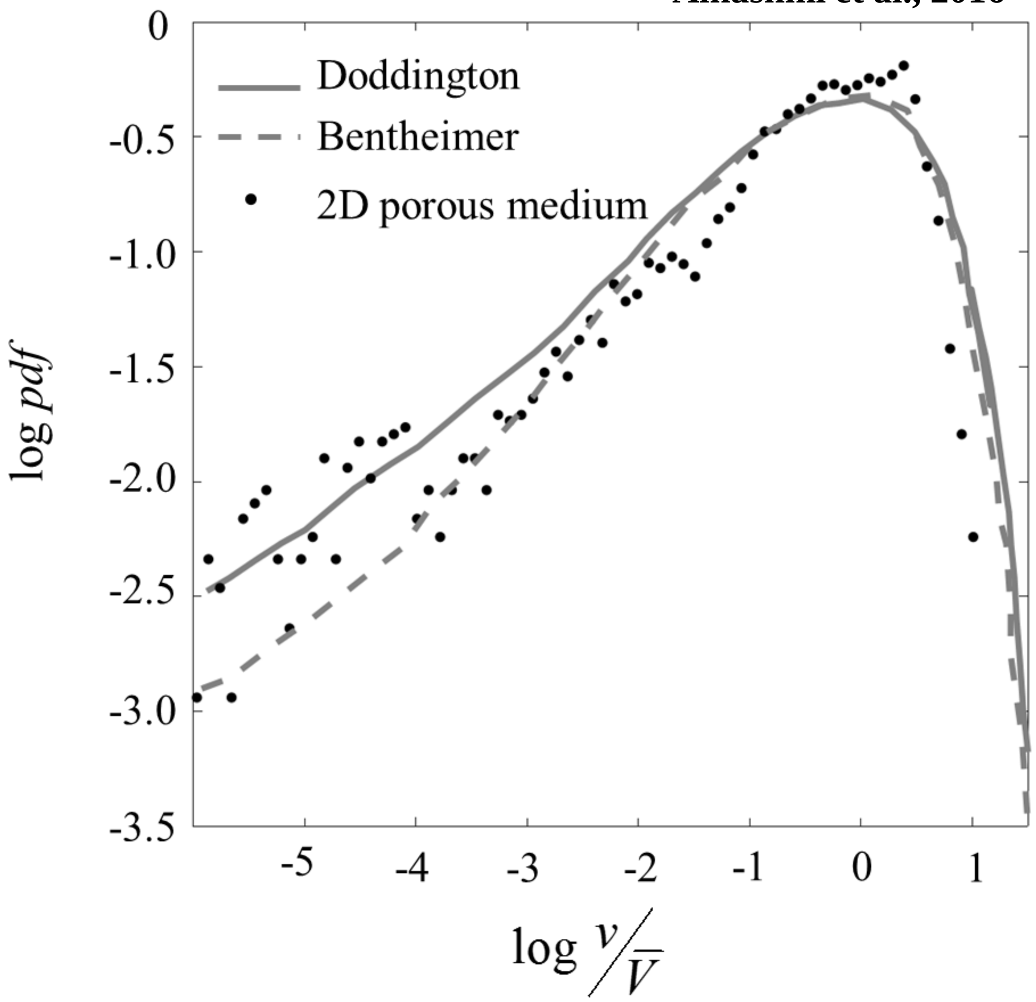
Case study



2D Periodic
× **N times**
$\phi = 0.59$

$\frac{v}{\overline{V}}$

Alhashmi et al., 2016



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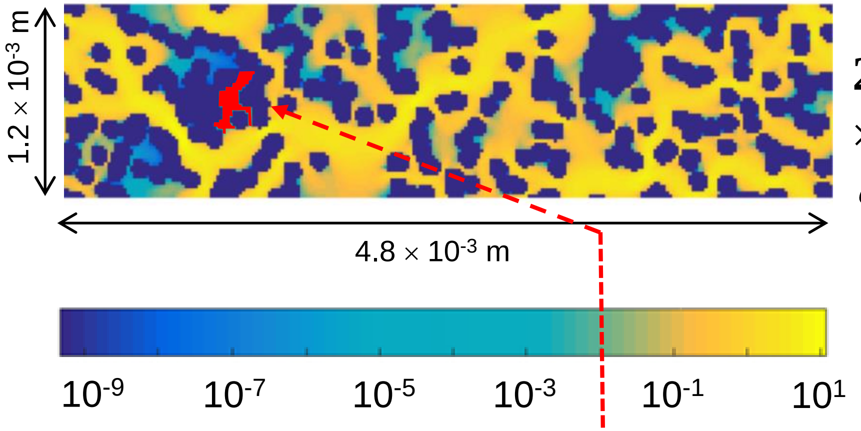
Case study



2D Periodic

× N times

$\phi = 0.59$

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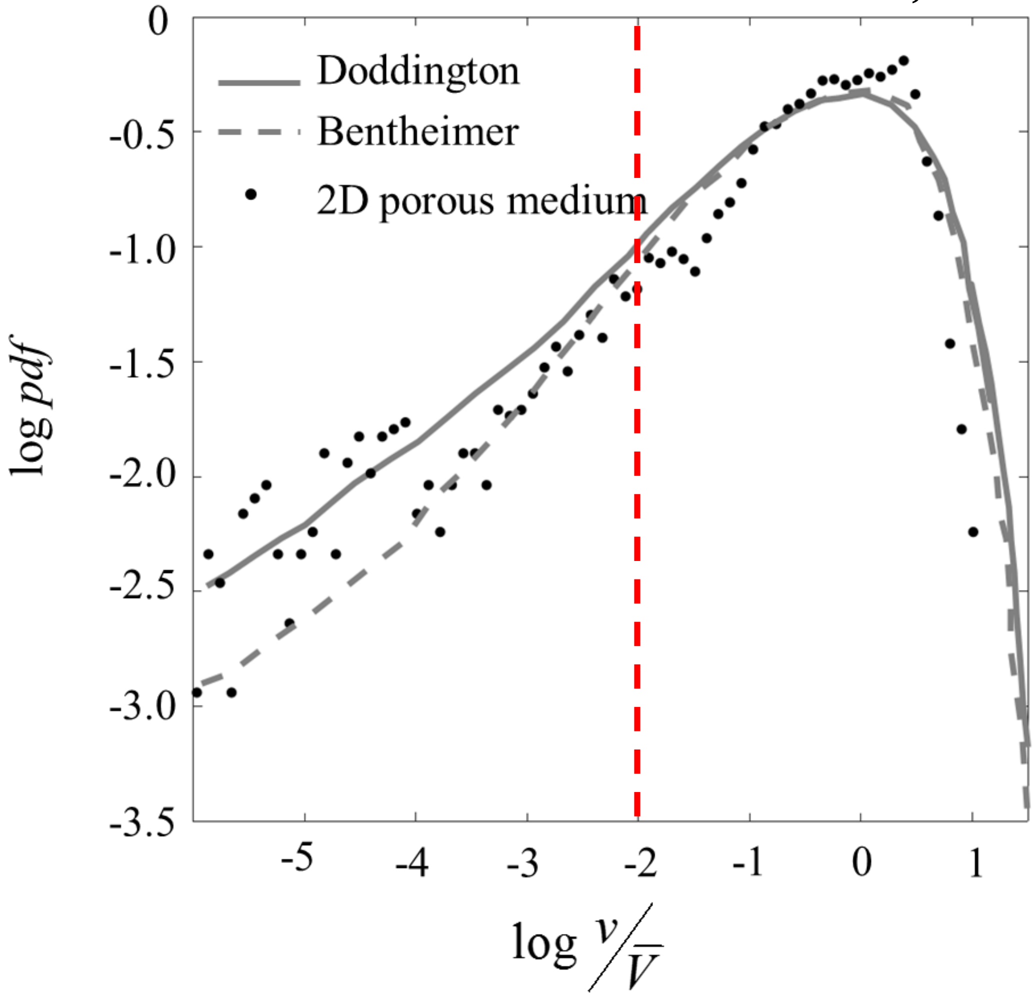
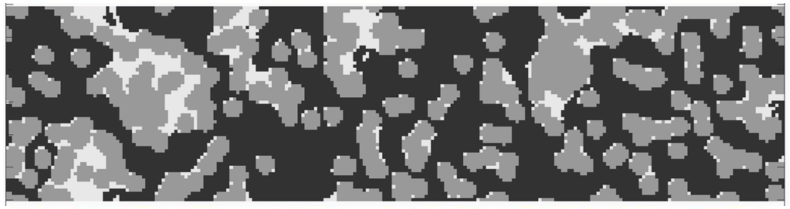
Alhashmi et al., 2016



Model calibration and validation

Case study and initial conditions

$v_{thr} = 10^{-2}$



$\phi_{HV} = 0.51 \quad \phi_{LV} = 0.08$

Model calibration and validation

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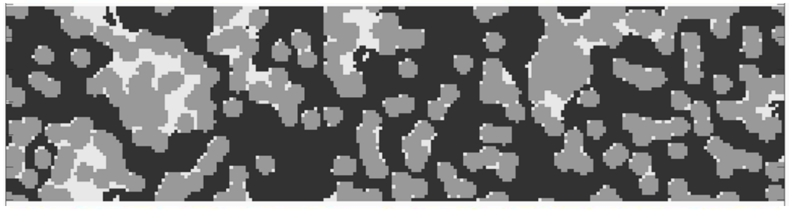

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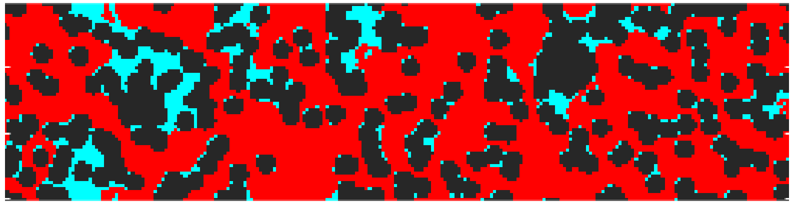
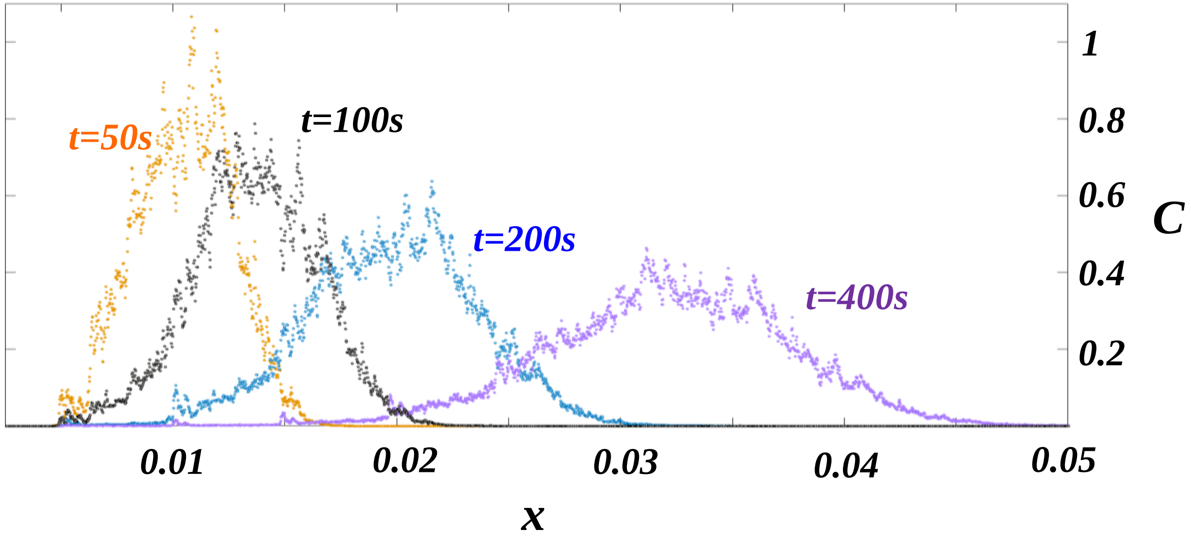
Initial conditions

S-HV





- **Pore-scale simulations using TDRW** (Russian et al., 2016)

Case study and initial conditions

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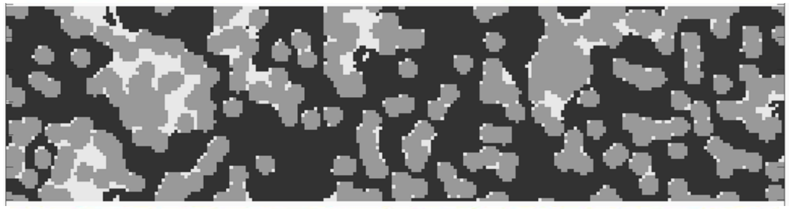

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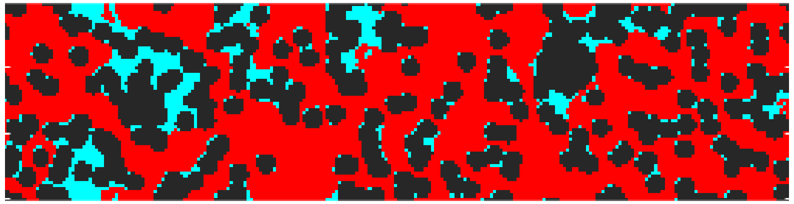
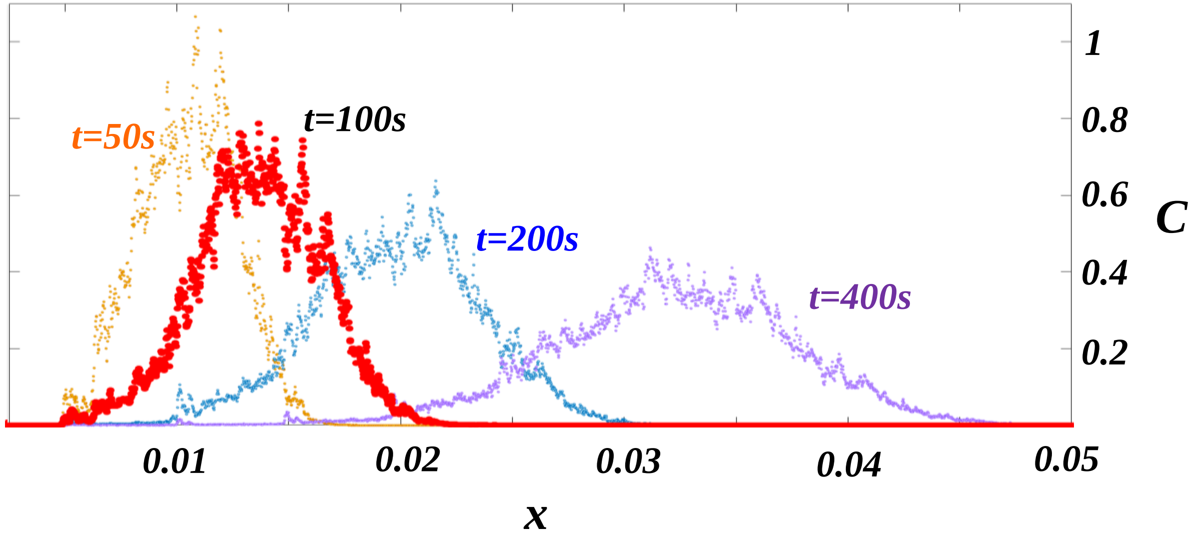


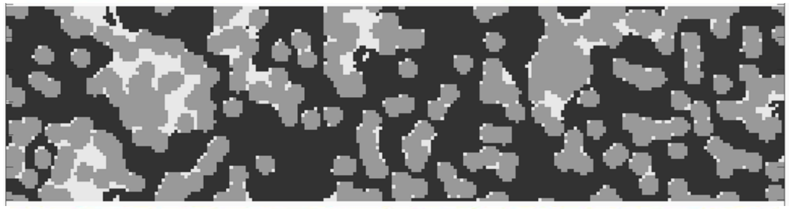


- **Pore-scale simulations using TDRW** **(Russian et al., 2016)**
- **Model Calibration using t = 100 s**

$$OBF = \sum \left[C(\hat{x}_i) - C_i^* \right]^2$$

Case study and initial conditions

$v_{thr} = 10^{-2}$



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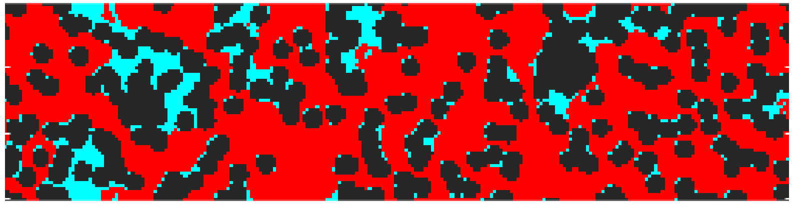
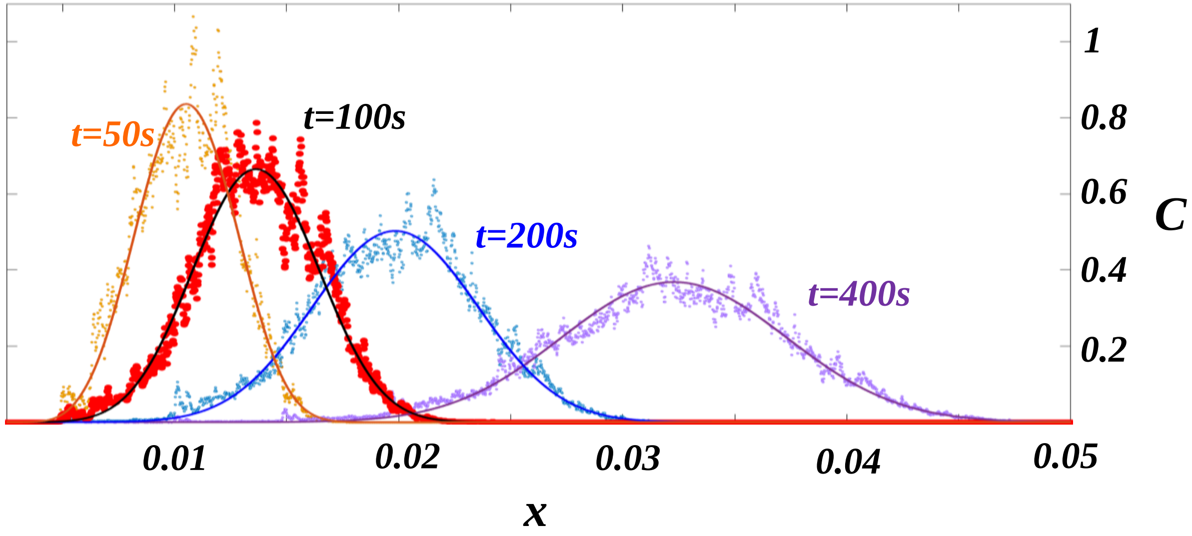




- **Pore-scale simulations using TDRW (Russian et al., 2016)**
- **Model Calibration using t = 100 s**

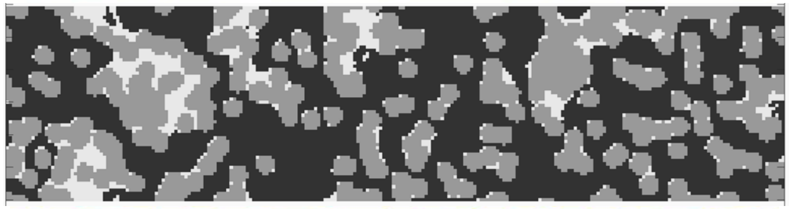
$$OBF = \sum \left[C(\hat{x}_i) - C_i^* \right]^2$$

L	R_D
743 μm	$10^{-1.011}$

Model calibration and validation

Case study and initial conditions

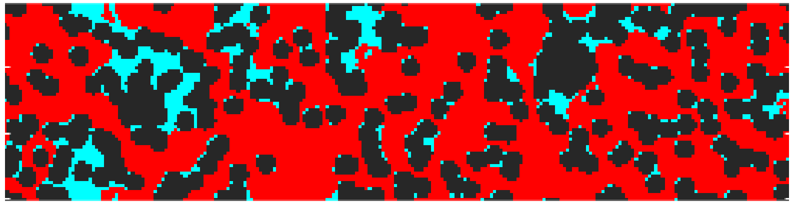
$v_{thr} = 10^{-2}$



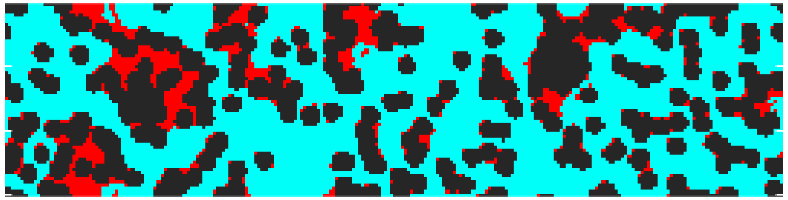
$\phi_{HV} = 0.51 \quad \phi_{LV} = 0.08$

Initial conditions

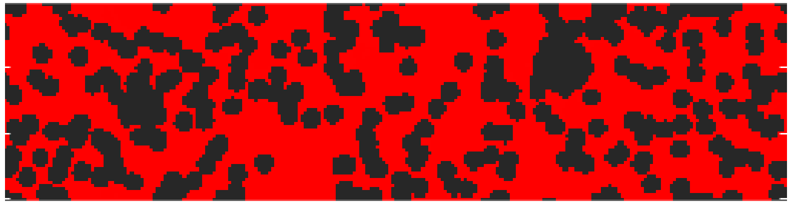
S-HV

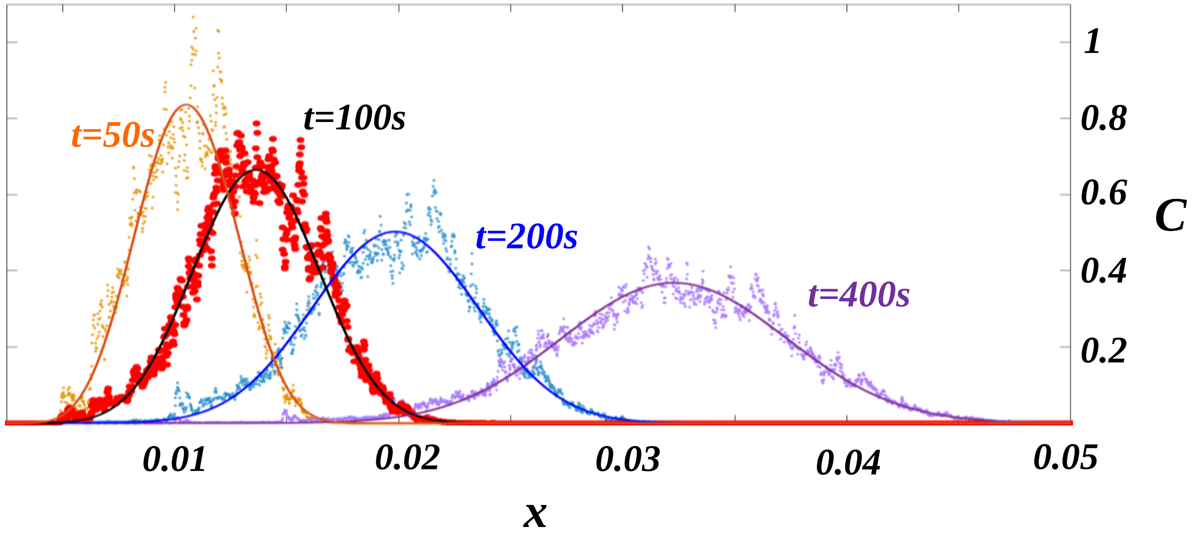


S-LV



S-ALL





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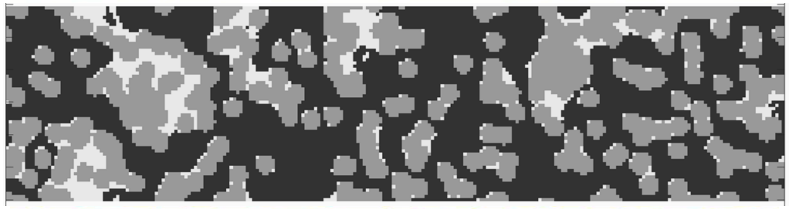

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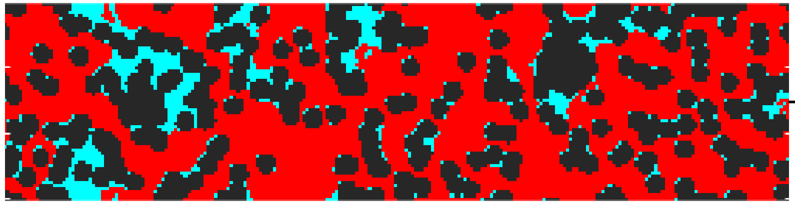
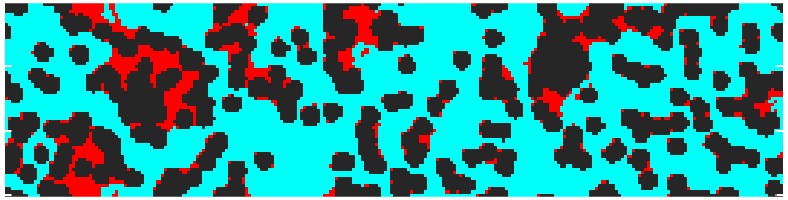
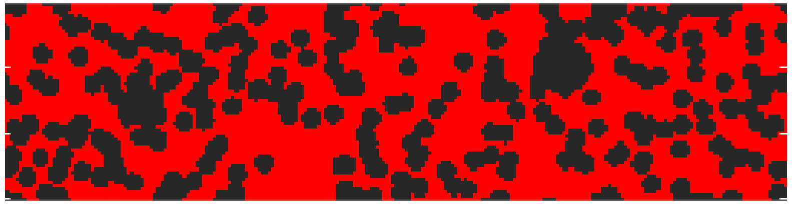
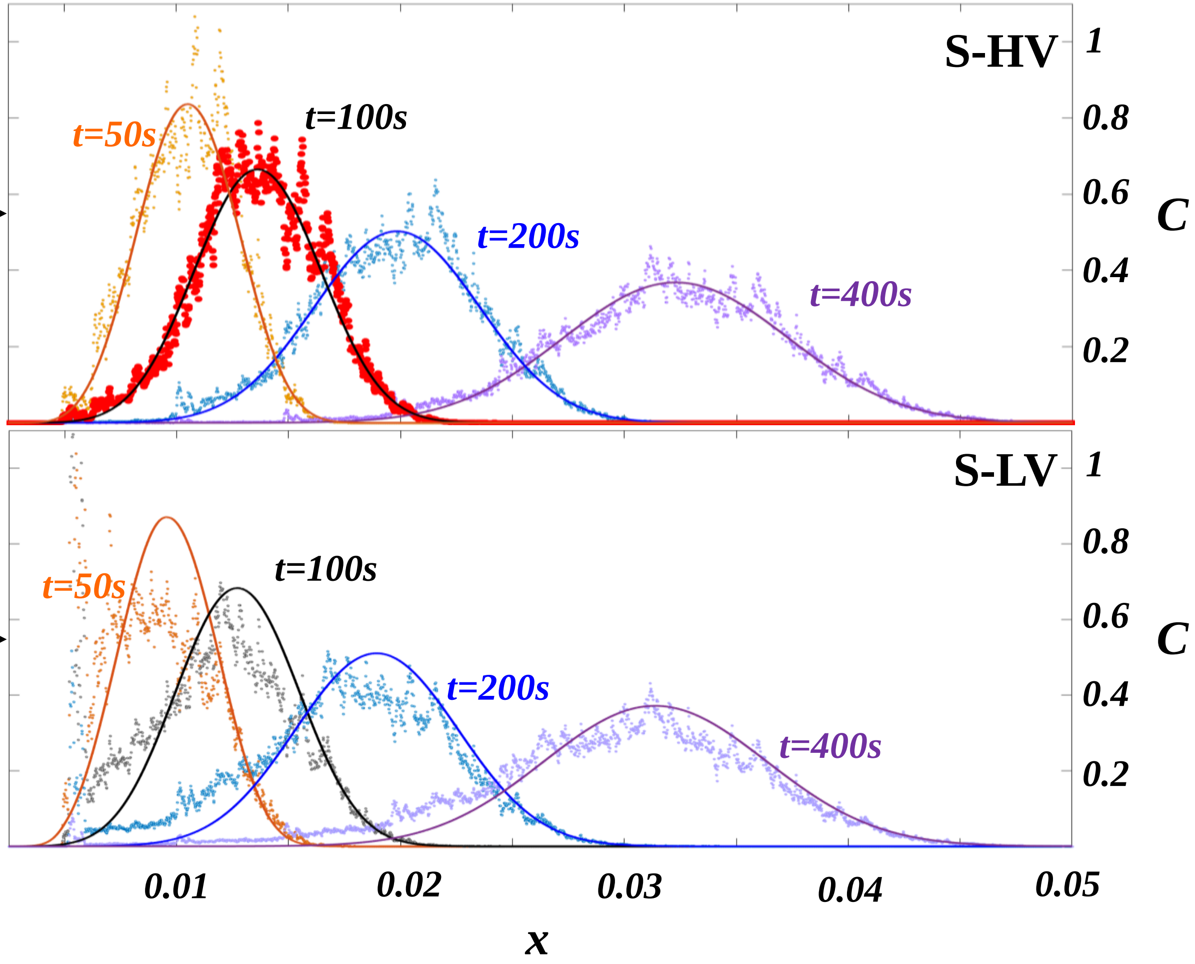


S-LV



S-ALL





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Sensitivity analysis (Razavi and Gupta, 2015; Pianosi et al., 2016)

- **Ranges**

$$L \in [80\mu m; 1200\mu m]$$

$$R_D \in [10^{-5}; 1]$$

- **Sampling**

N=1000 Monte Carlo realizations

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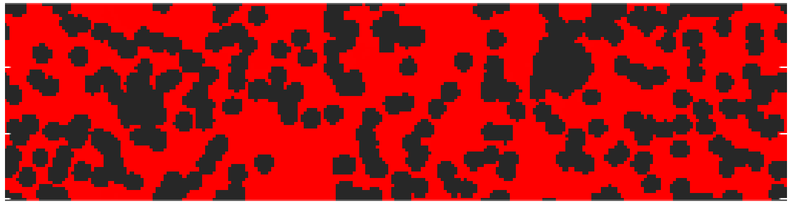

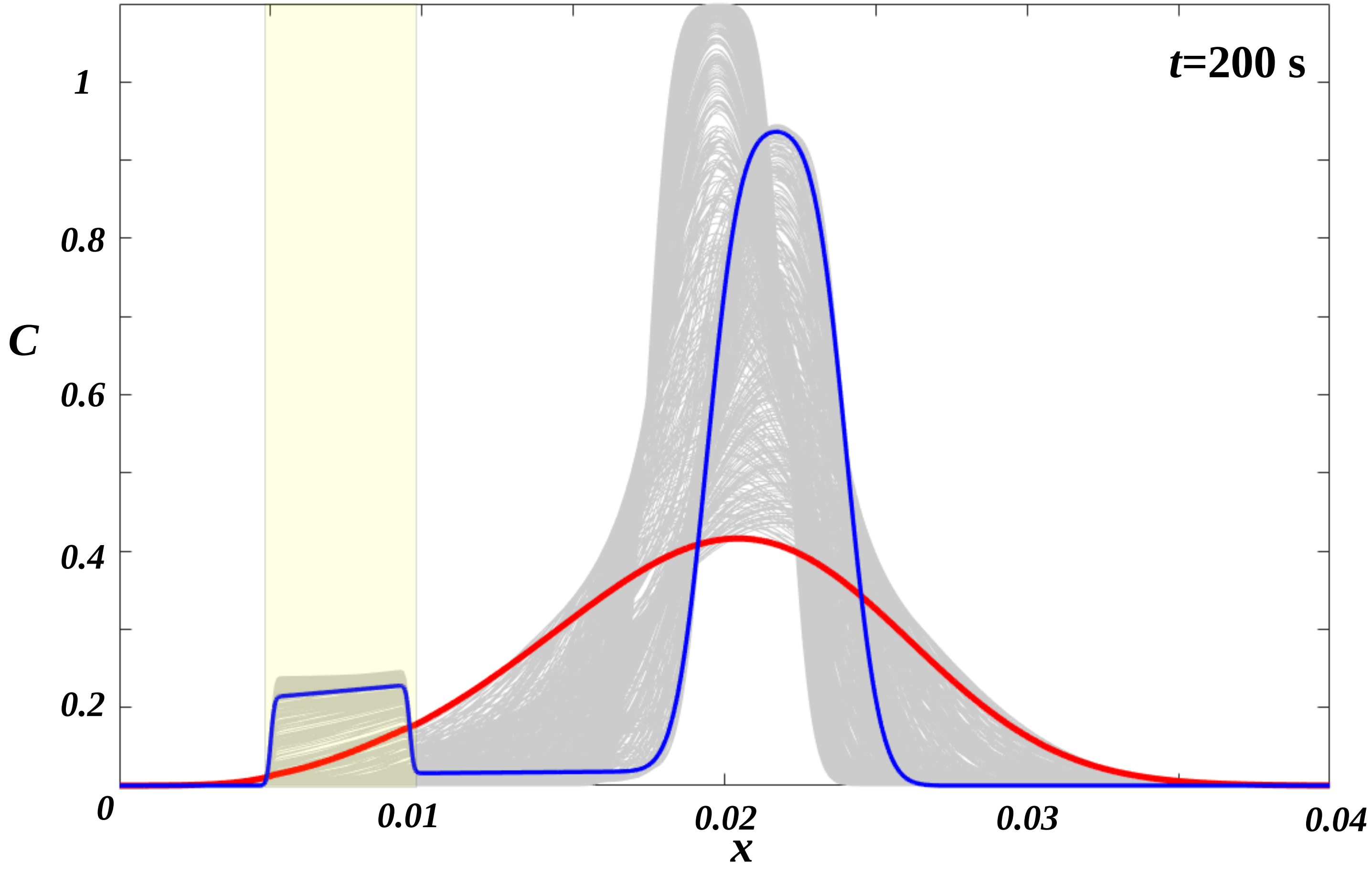

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- **Target Variables**

Profile Spread

$$\sigma^2(\hat{t}) = \int_D [\hat{x} - \mu(\hat{t})]^2 C_n(\hat{x},\hat{t})d\hat{x}$$

Profile Skewness

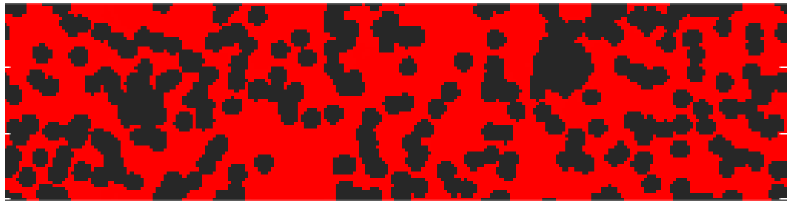
$$\gamma(\hat{t}) = \frac{\int_D [\hat{x} - \mu(\hat{t})]^3 C_n(\hat{x},\hat{t})d\hat{x}}{\sigma^3(\hat{t})}$$

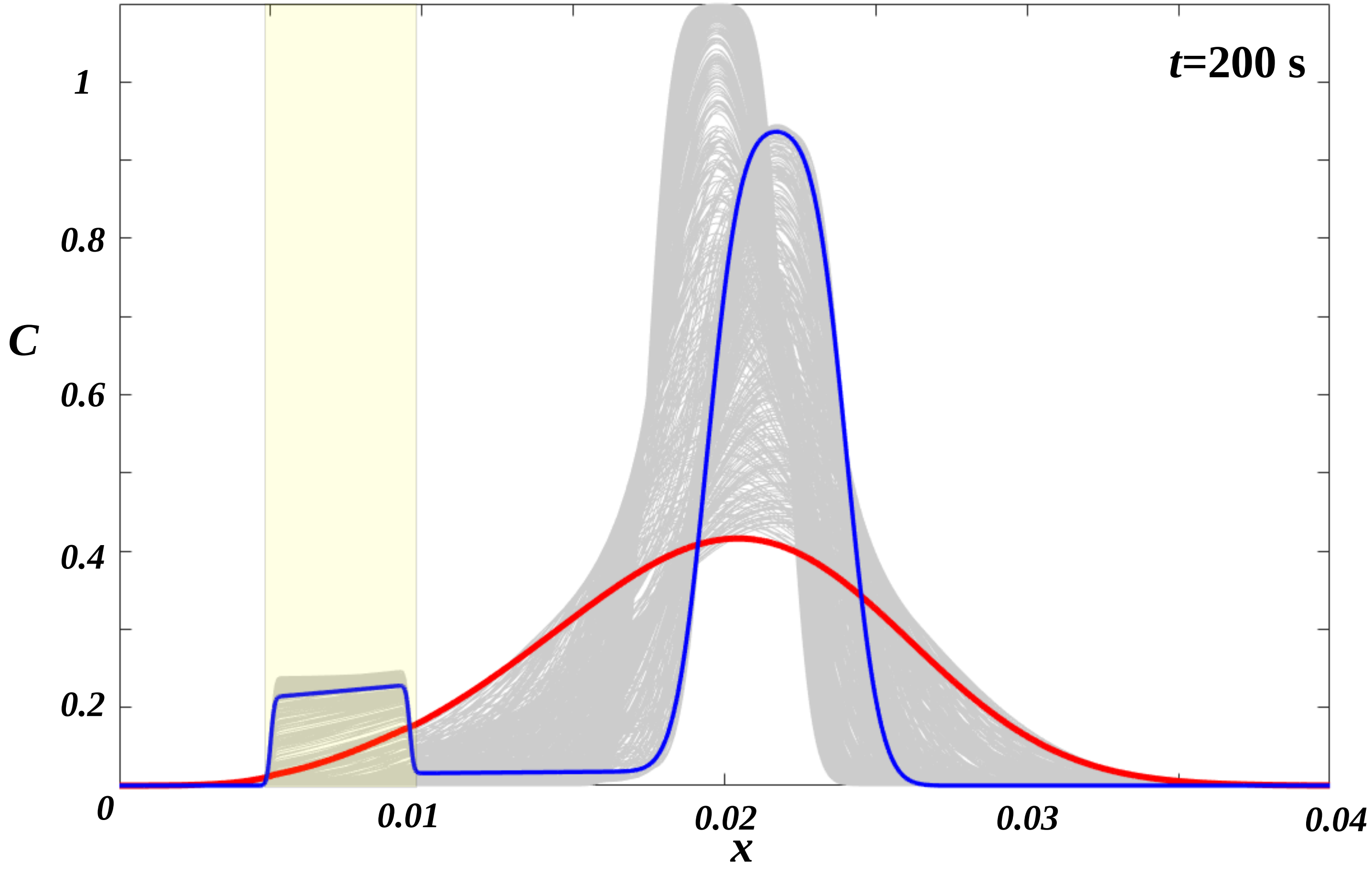
- ***Compute the Sobol' indices***

$$SI(\sigma^2)_L + SI(\sigma^2)_{RD} + SI(\sigma^2)_{L,RD} = 1$$

$$SI(\gamma)_L + SI(\gamma)_{RD} + SI(\gamma)_{L,RD} = 1$$

S-ALL





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The contribution to the variance of the profile spread given by the variability of L

Sensitivity analysis (Razavi and Gupta, 2015; Pianosi et al., 2016)

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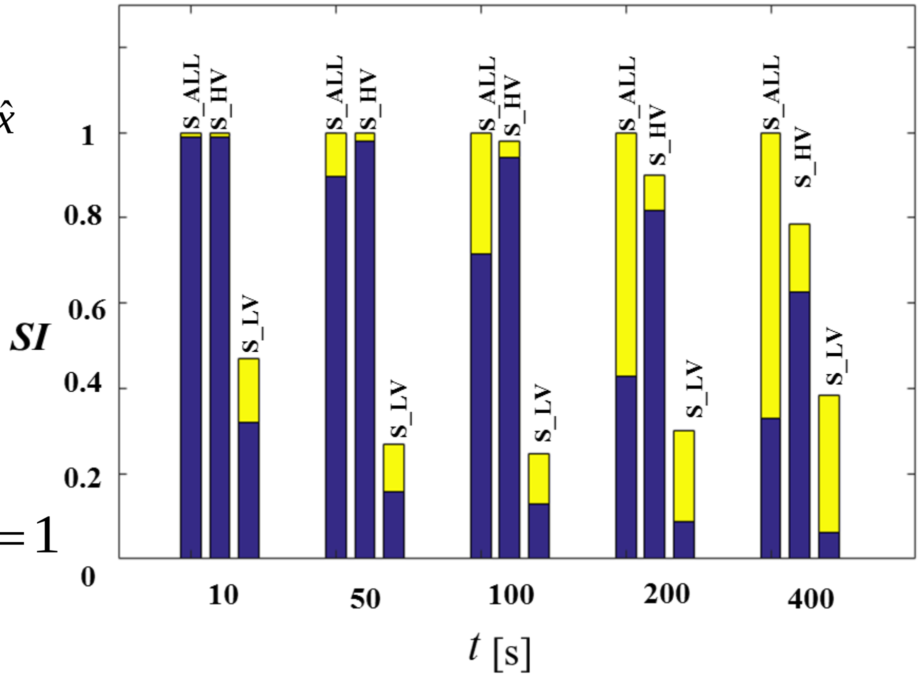
Sensitivity of solute profile SPREAD



Model Calibration via Sensitivity Analysis

Sensitivity analysis (Razavi and Gupta, 2015; Pianosi et al., 2016)

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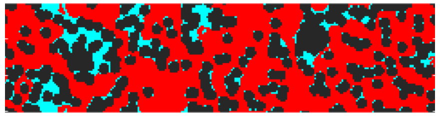
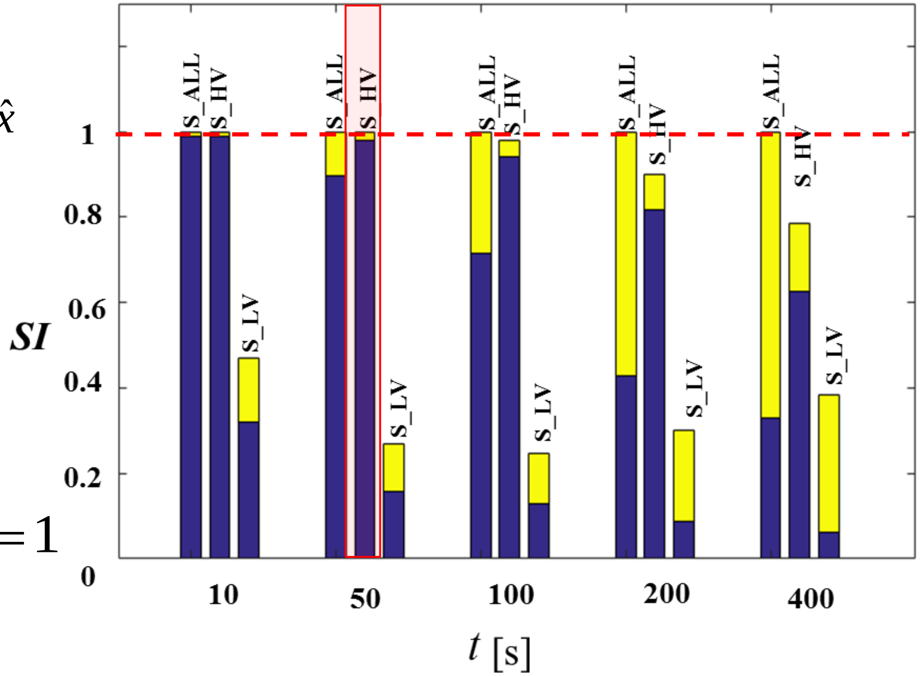


S-HV Profile Spread at *t* =50 s sensitive to *L*

$$P1 = \left| 1 - \frac{\sigma^2_{HV}(50s)}{\sigma^2_{PS}} \right|$$

Sensitivity of solute profile SPREAD



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POLITECNICO MILANO 1863

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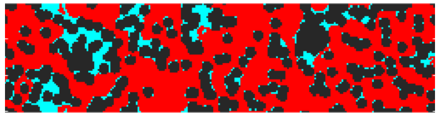

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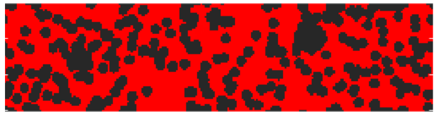
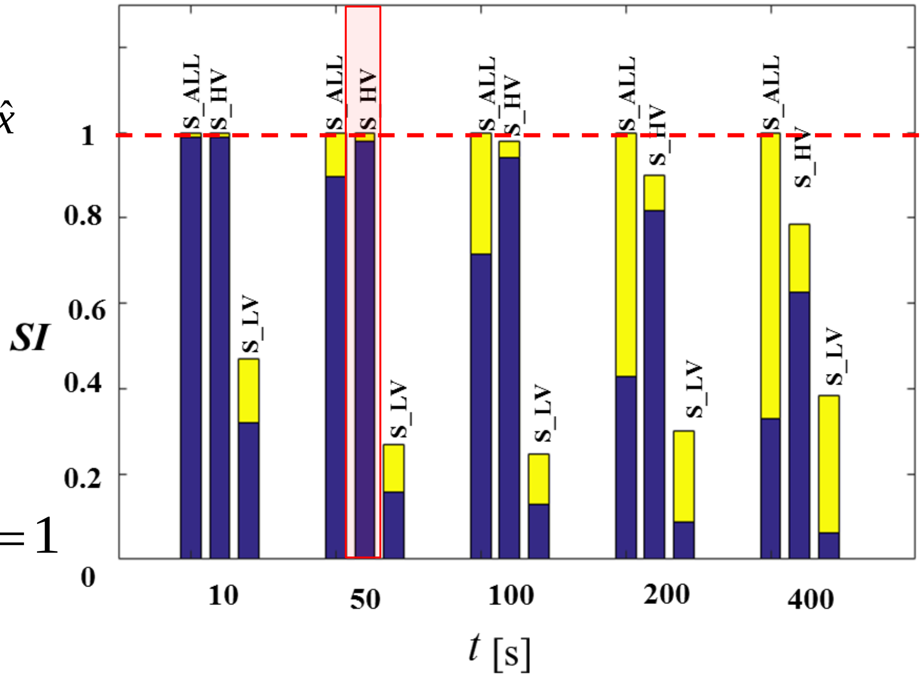


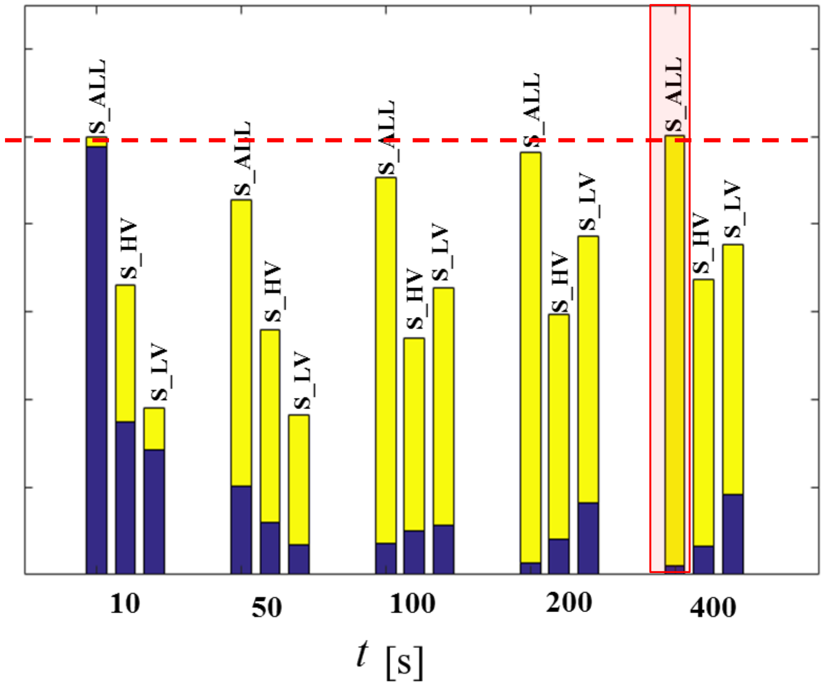
S-ALL Profile Skewness at *t* =400 s sensitive to R_D

$$P2 = \left| 1 - \frac{\gamma_{ALL}(400s)}{\gamma_{PS}} \right|$$

Sensitivity of solute profile SPREAD



Sensitivity of solute profile SKEWNESS



Sensitivity analysis (Razavi and Gupta, 2015; Pianosi et al., 2016)

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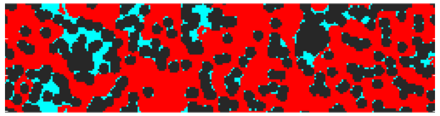

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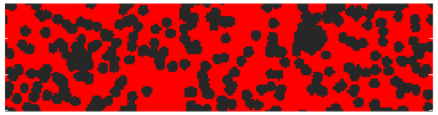

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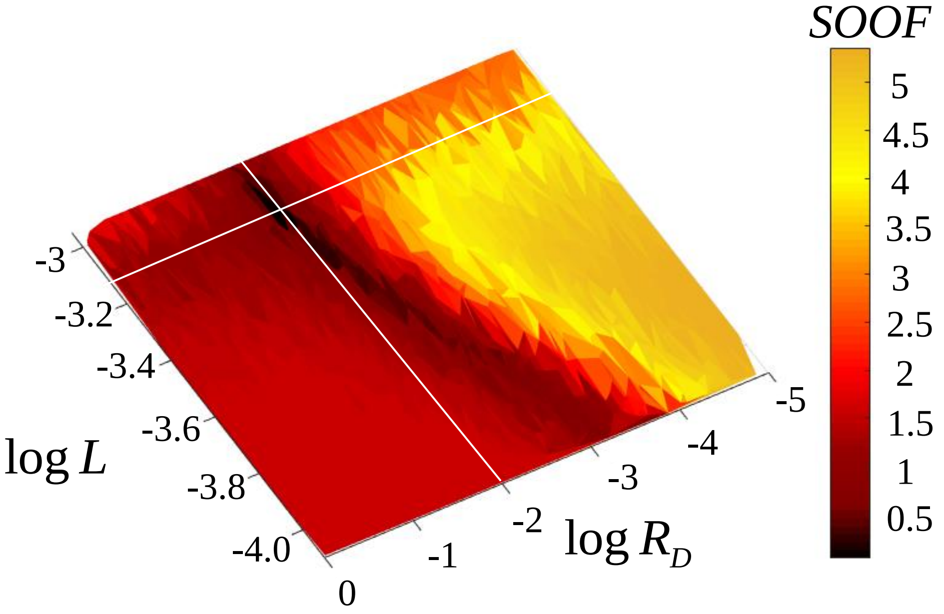

Definition of a new calibration criterion

$$SOOF = P1 + P2$$

Model Validation with *SOOF* criterion

SOOF Calibration

L	R_D
673.4 μm	$10^{-1.9972}$

OBF Calibration

743 μm	$10^{-1.011}$

Model Validation with *SOOF* criterion

SOOF Calibration

L	R_D
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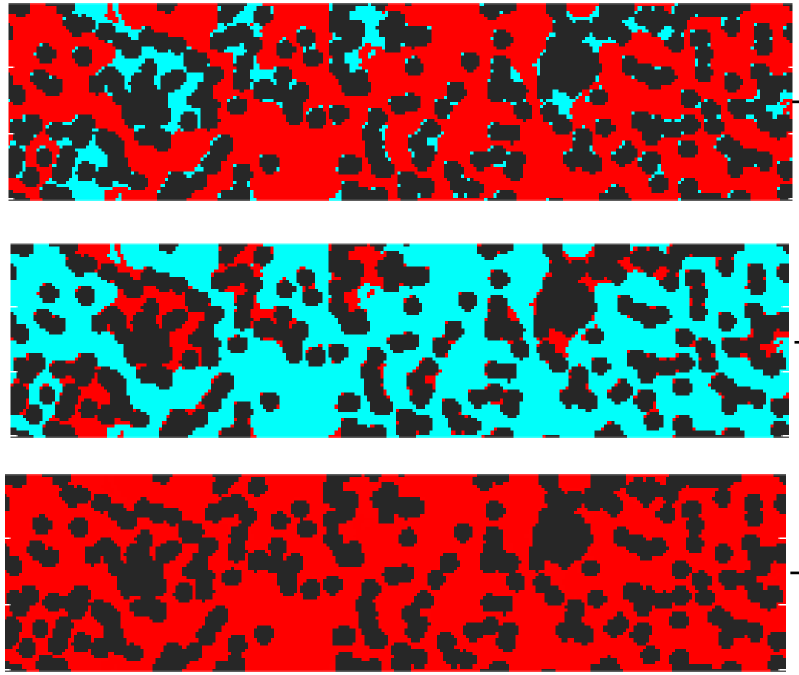
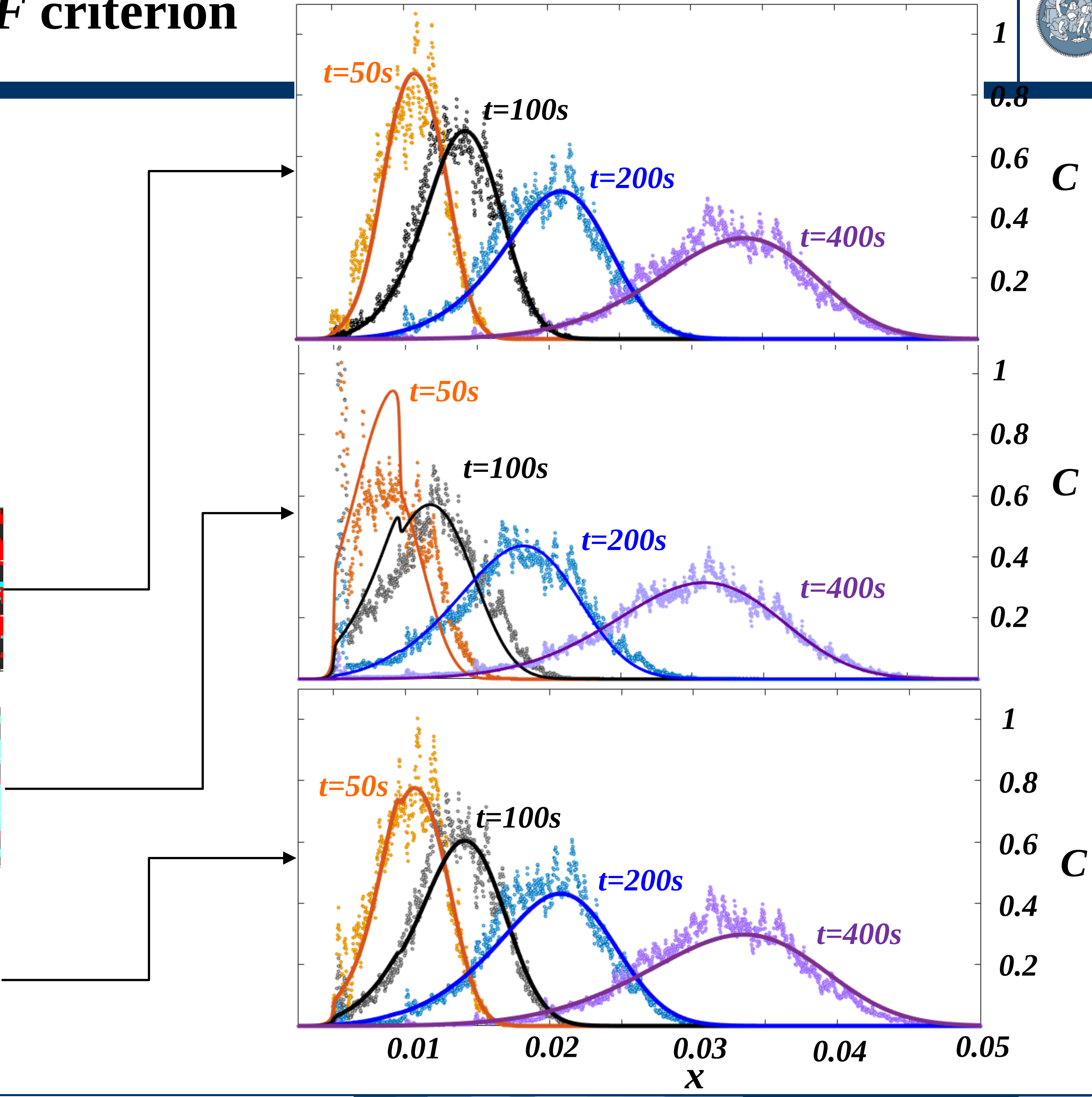
Initial conditions

S-HV

S-LV

S-ALL





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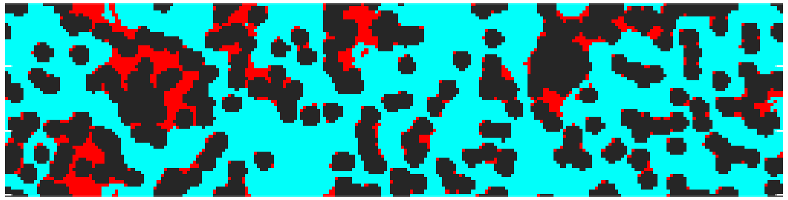

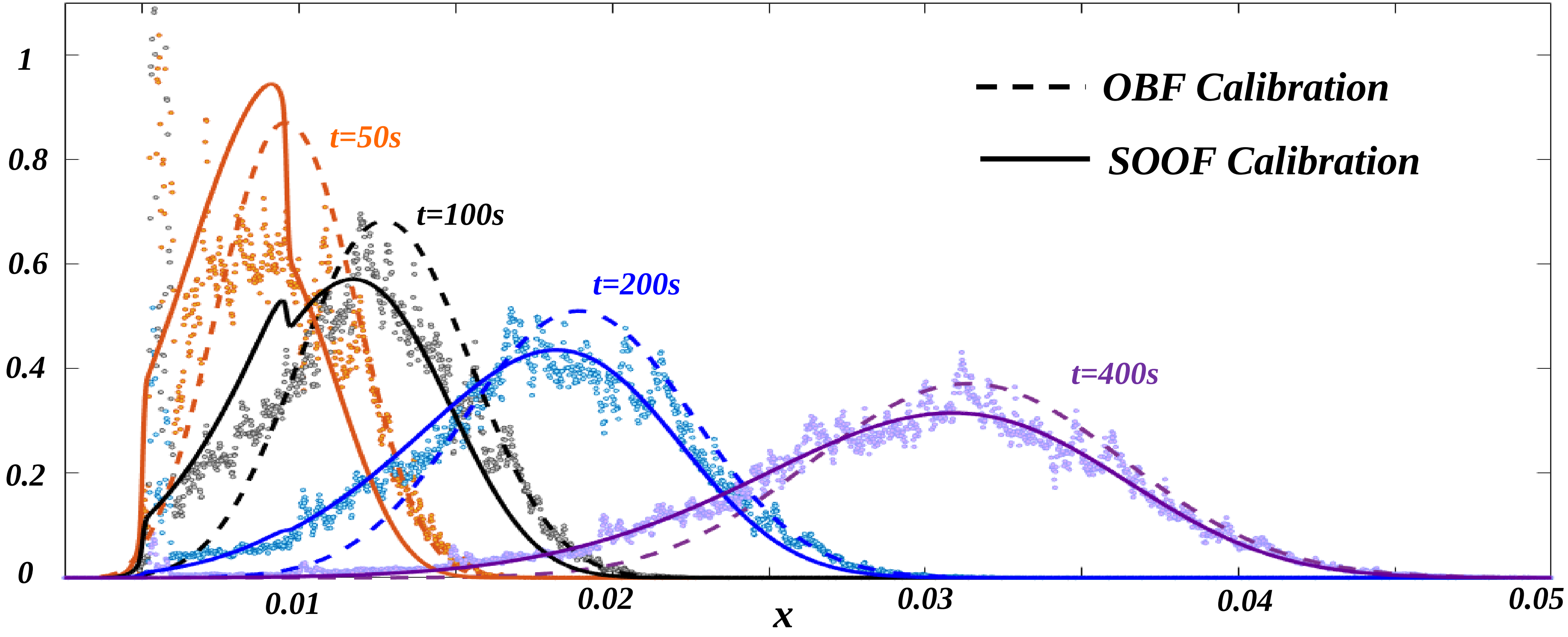

Model Validation with *SOOF* criterion

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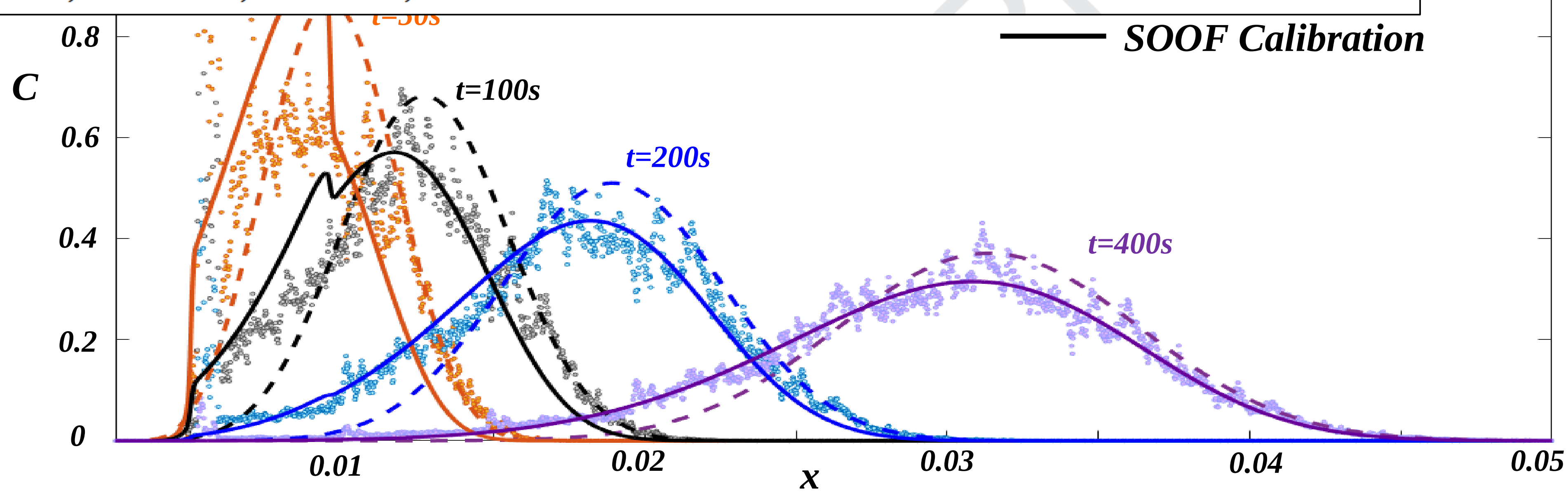
A double-continuum transport model for segregated porous media: Derivation and sensitivity analysis-driven calibration

G. Ceriotti[a,*], A. Russian[a], D. Bolster[b], G. Porta[a]



On going: R_D and its link to porous geometry

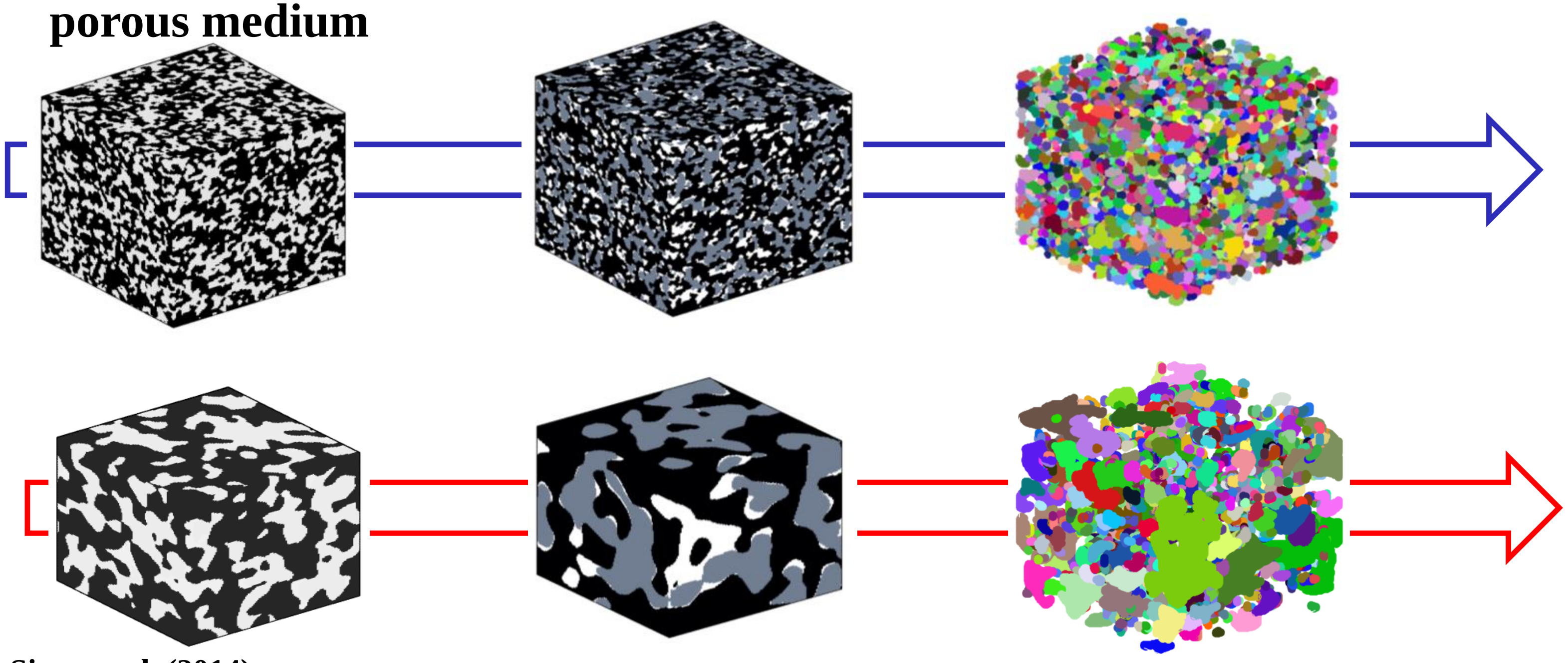
Can we estimate the value of R_D directly from the geometry structure of immobile regions?

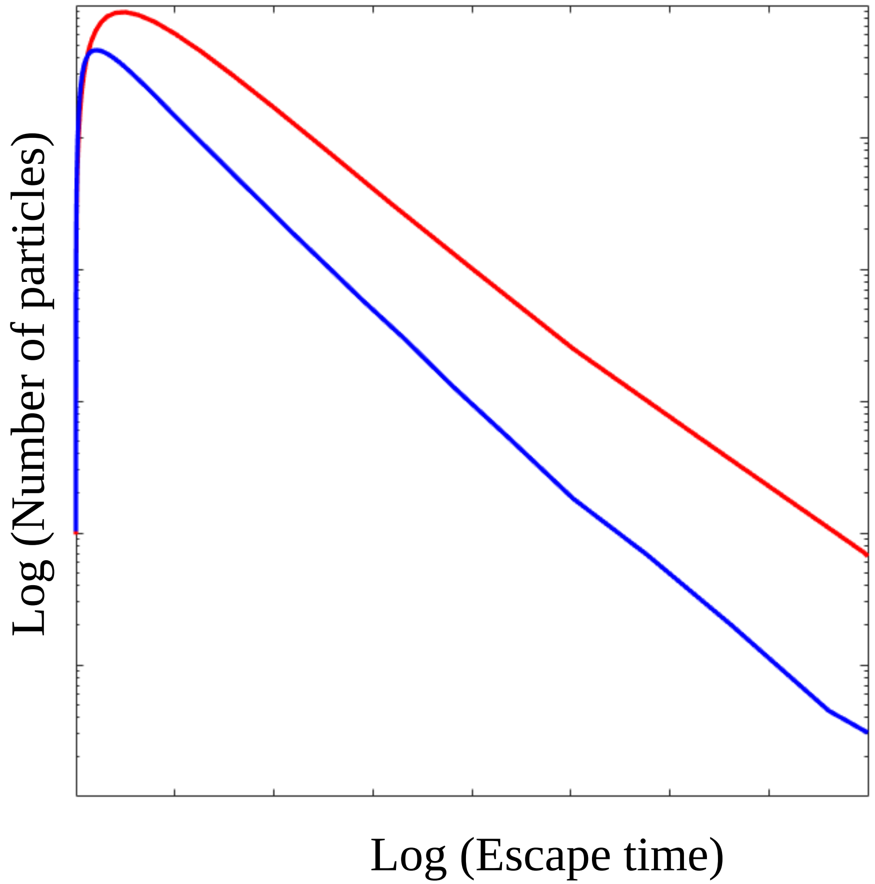
Generation of a porous medium

Define a velocity threshold

Analysis of the shape, connectivity and dimension of the low-velocity regions

Particle tracking simulations of the escape time





Siena et al. (2014)

Acknowledgments

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UNIVERSITY OF NOTRE DAME

Anna Russian

Diogo Bolster

Giovanni Porta

EU and MIUR for funding, in the frame of the collaborative international Consortium (**WE-NEED**) financed under the ERA-NET WaterWorks2014 Co- funded Call

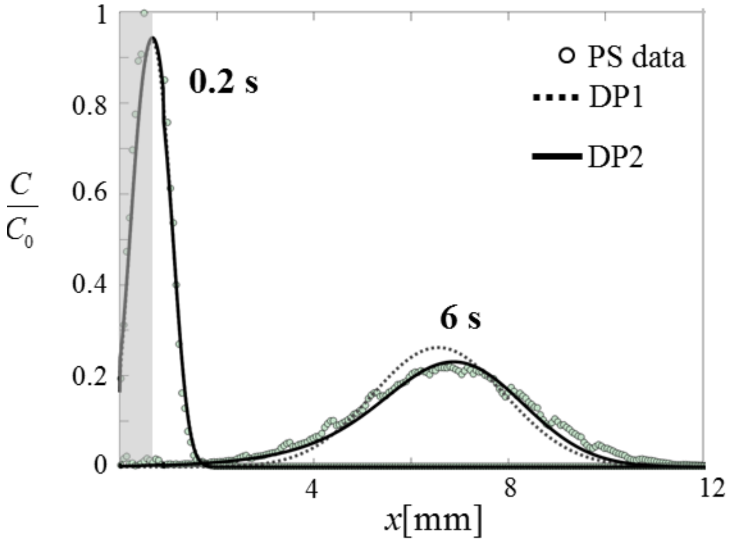
WE-NEED
WatEr NEEDs, Availability, Quality and Sustainability

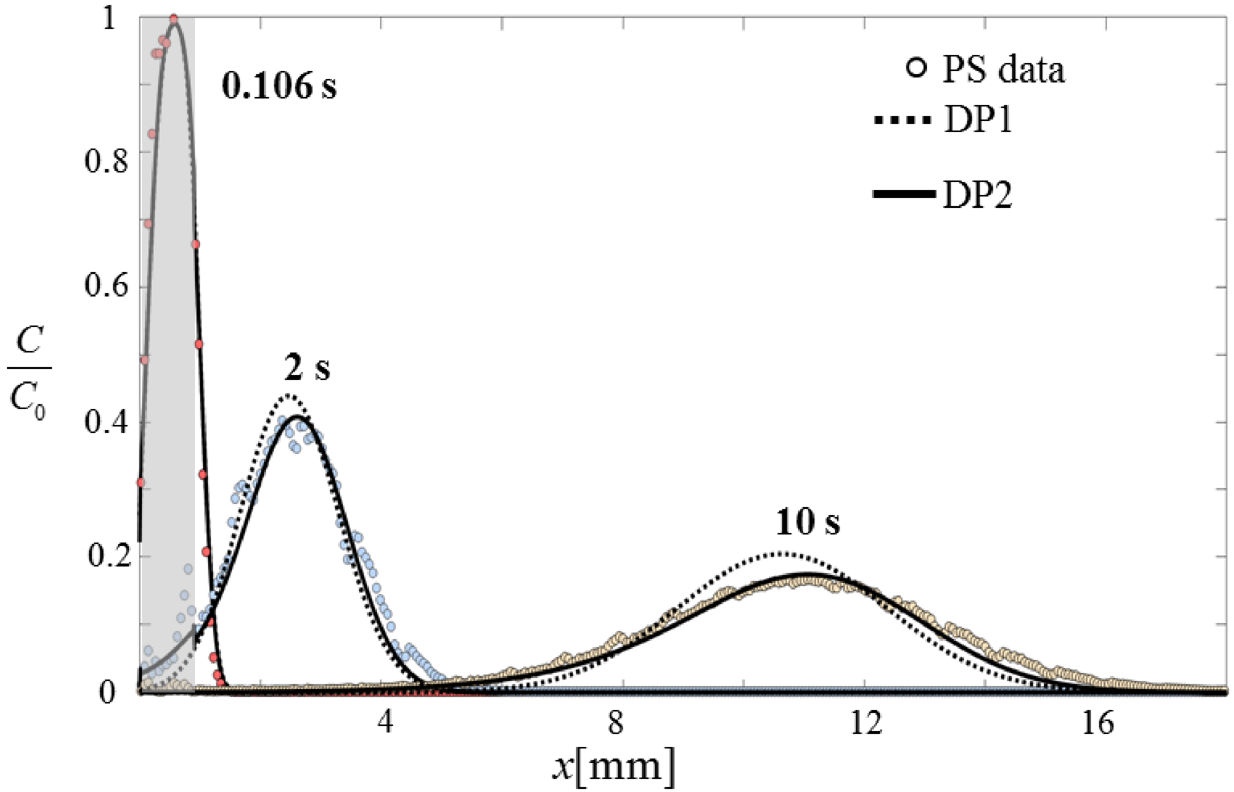
Water JPI

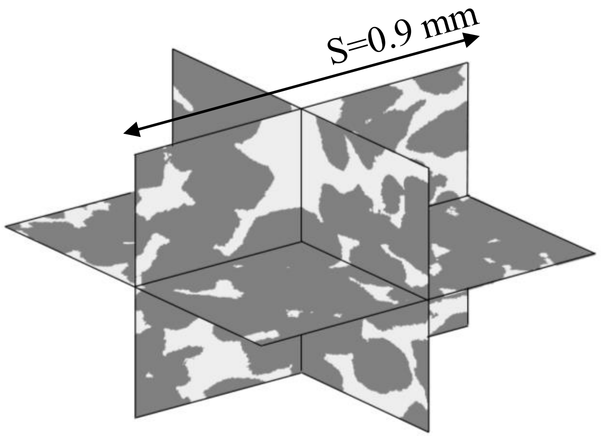
Water 2014 Works

On going: Starting to test it on 3D porous media

Is the model performing well on 3D case studies?







X-ray scanned 3D sandstone

(Bijeljic et al., 2011)

ϕ	0.214
ϕ_m	0.199
ϕ_{im}	0.015

(Manually) Estimated parameters	
L	100.45 µm
R_D	0.0017