27th Oil Shale Symposium, Golden, CO
15-19 October 2007

Multiscale Modelling of Flow and Solute Transport in the Piceance Basin:

Development of Efficient Techniques for Representing Rate-limited Mobilization of Potential Groundwater Contaminants

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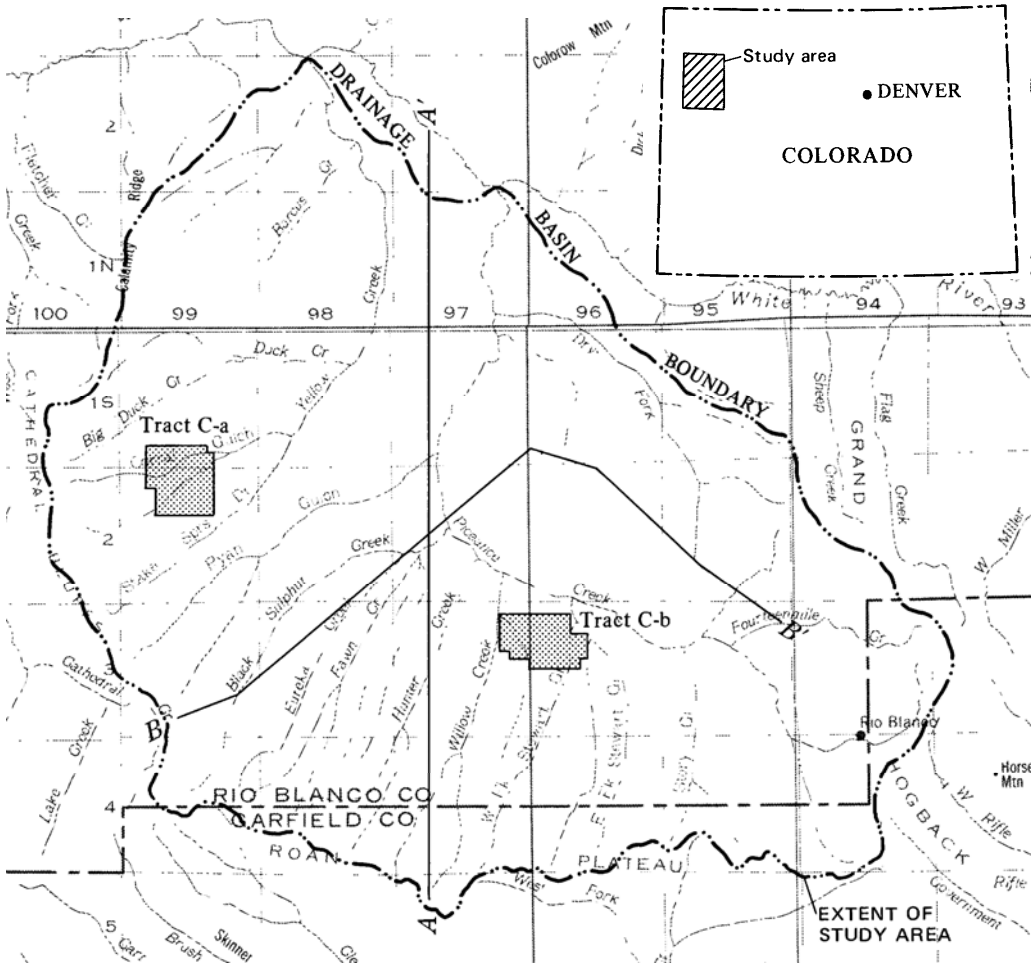
Piceance Basin of Northwestern Colorado

- 70 km long, average width of 30 km
- Surface area of about 2300 km^2



From Weeks et al. (1974)

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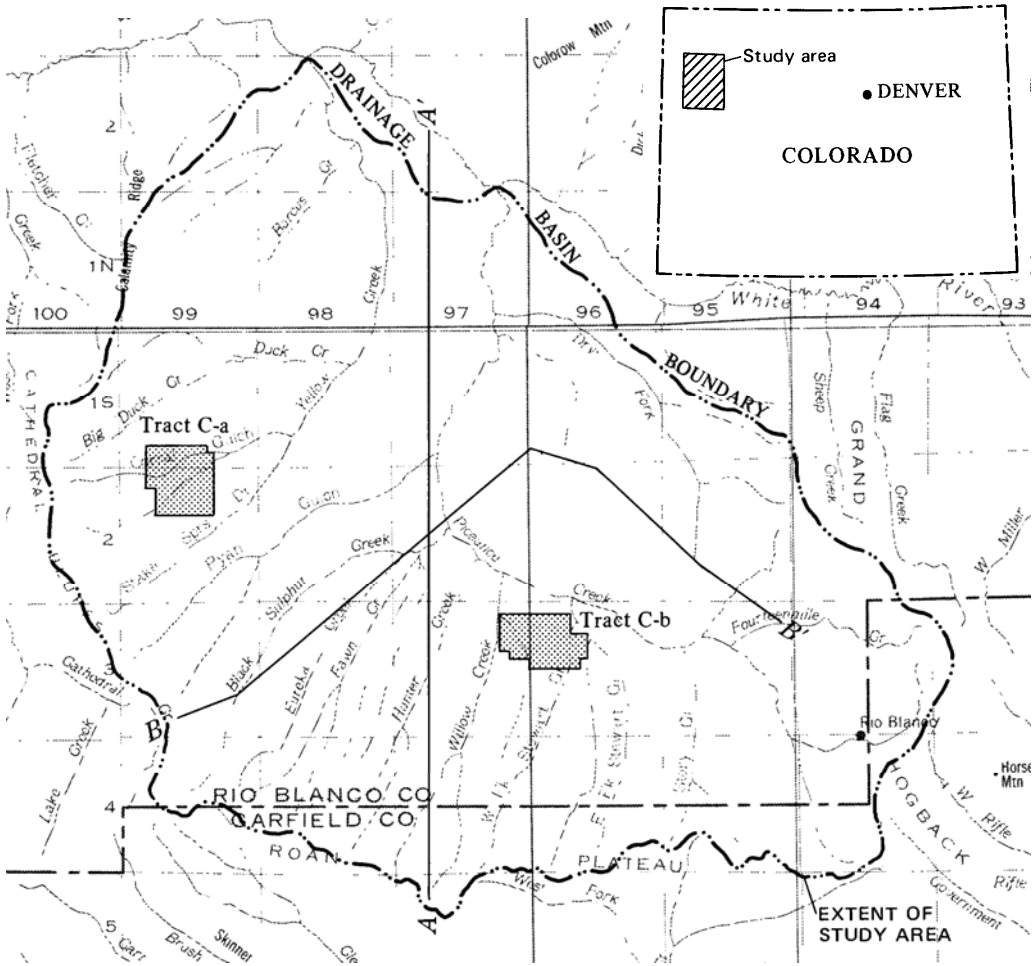

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Piceance Basin of Northwestern Colorado

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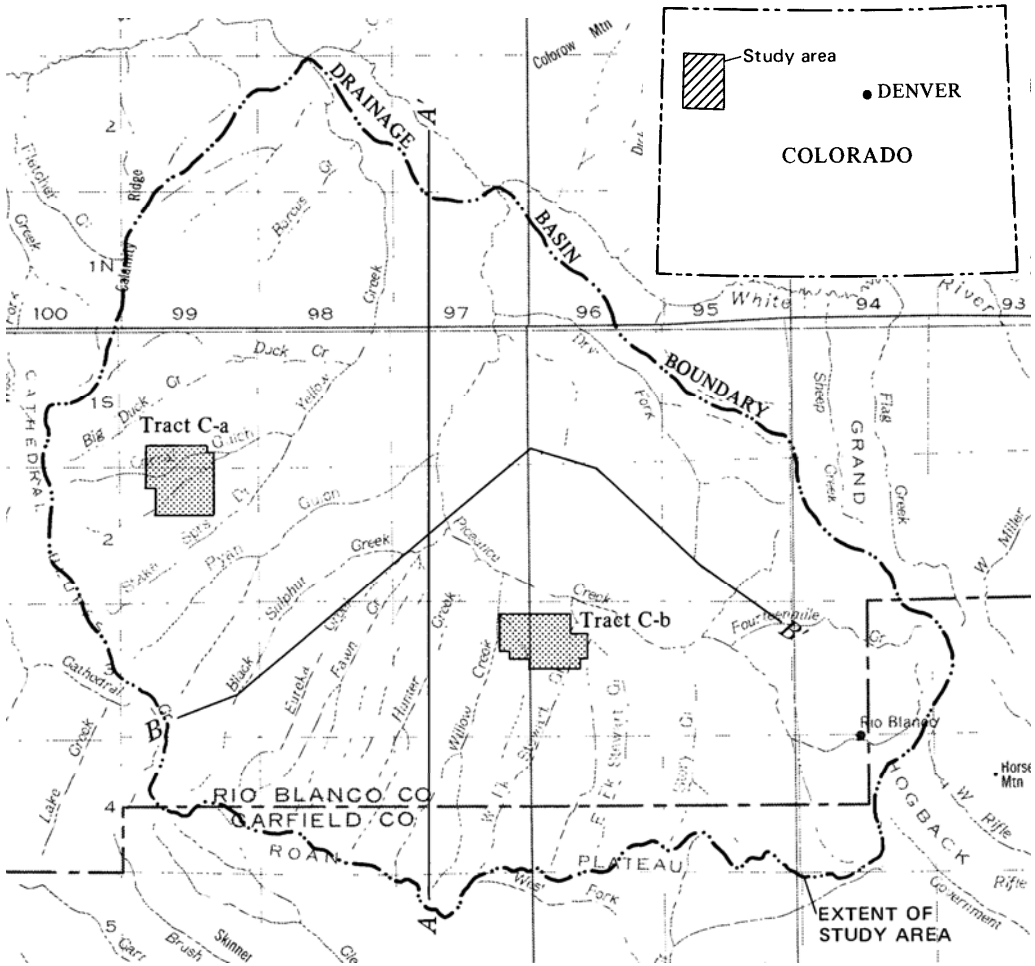
- World's largest deposit of oil shale
- Intense in situ mining activities expected in the next century



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Potential Environmental Impacts of In Situ Oil Shale Mining

- Increase in soil temperature
- Release of large amounts of organic components
- Changes in the chemistry of the soil
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- Need to understand the fundamental processes involved and develop predictive modelling tools for surface and subsurface water quality

Objectives of this research

- Develop an understanding of the effect of local-scale heterogeneities on flow and solute transport at the basin scale

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Outline

- Upscaling methods for flow and solute transport
- Our approach : FEHM and the GDPM capability
- Characterizing heterogeneity in the Piceance basin
- Preliminary results : the Mahogany zone
- Future work

Upscaling methods for flow and solute transport

The need for upscaling methods (1)

Modelling of flow and transport at the basin scale

Upscaling methods for flow and solute transport

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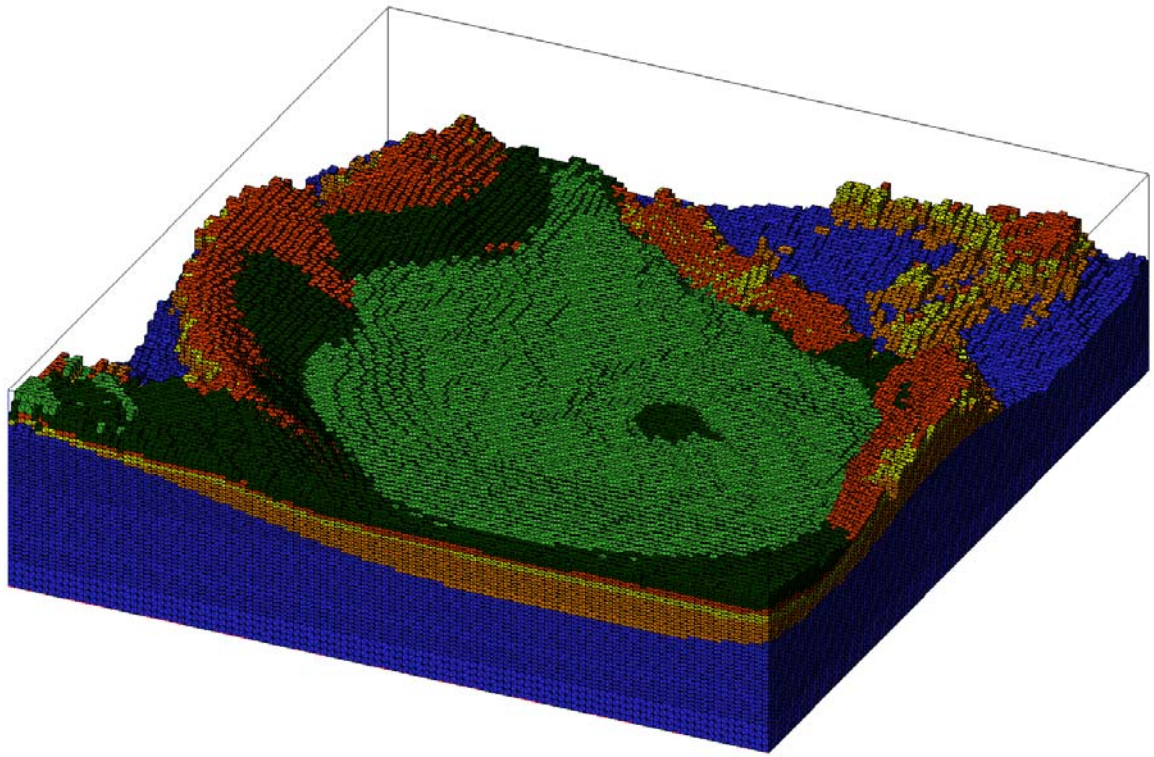
Modelling of flow and transport at the basin scale

7 layers hydrogeologic model



697,323 nodes - 500 x 500 x 25-50 m spacing

From http://meshing.lanl.gov/proj/OIL_SHALE_Piceance/

Upscaling methods for flow and solute transport

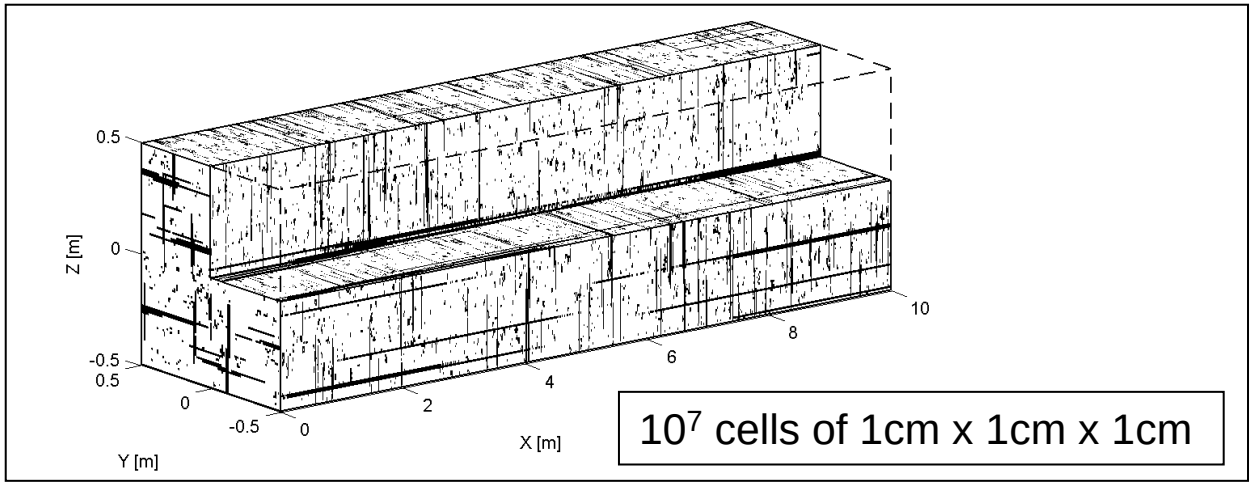
The need for upscaling methods (2)

Detailed modelling of flow and transport in heterogeneous media

Upscaling methods for flow and solute transport

The need for upscaling methods (2)

Fractured medium



10^7 cells of 1cm x 1cm x 1cm

Detailed modelling of flow and transport in heterogeneous media

Upscaling methods for flow and solute transport

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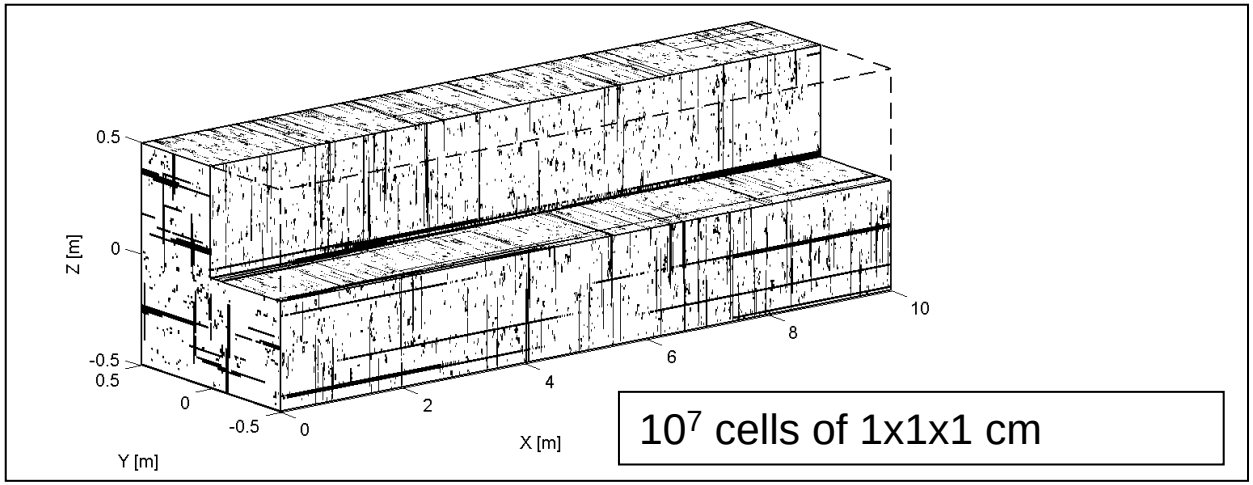
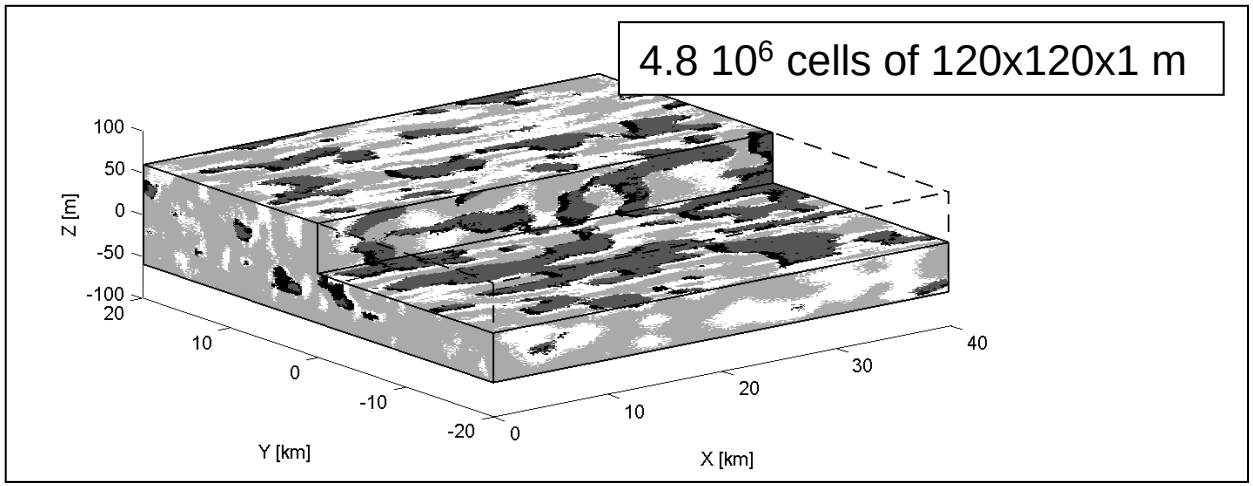
Detailed modelling of flow and transport in heterogeneous media

Heterogeneous porous medium



10^7 cells of 1x1x1 cm



$4.8\ 10^6$ cells of 120x120x1 m

Upscaling methods for flow and solute transport

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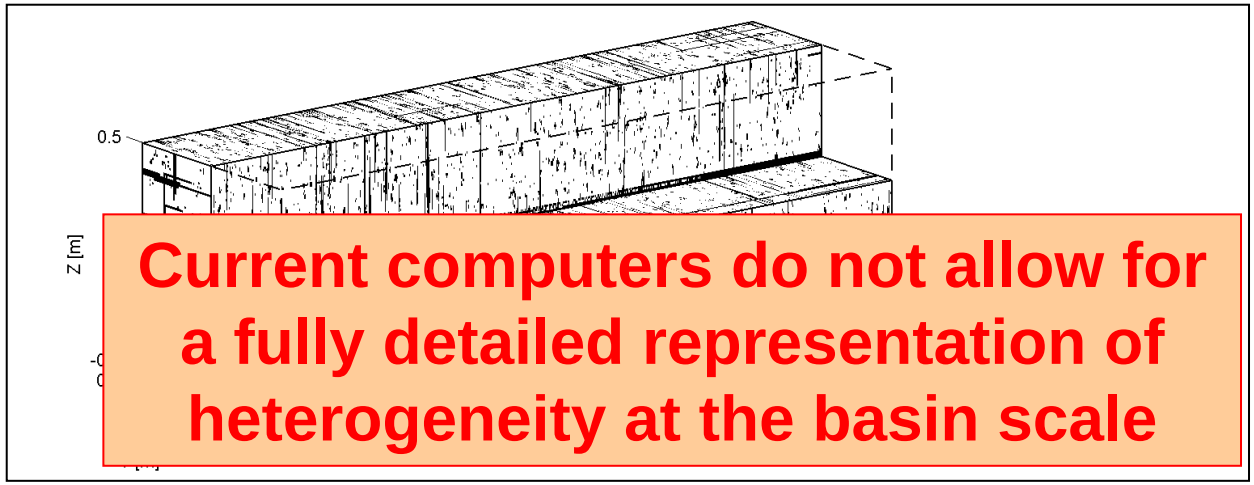
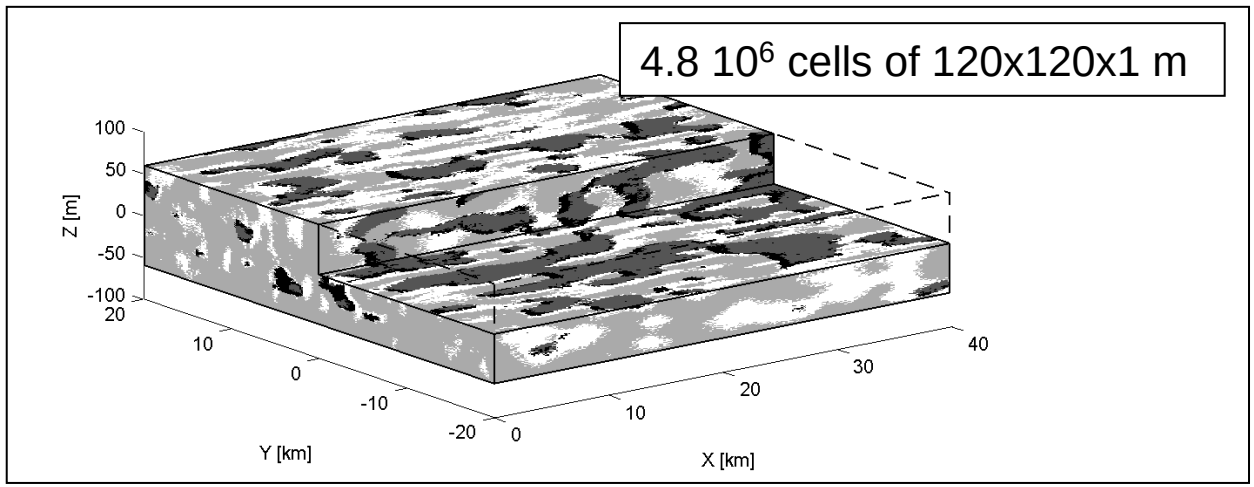


Current computers do not allow for a fully detailed representation of heterogeneity at the basin scale



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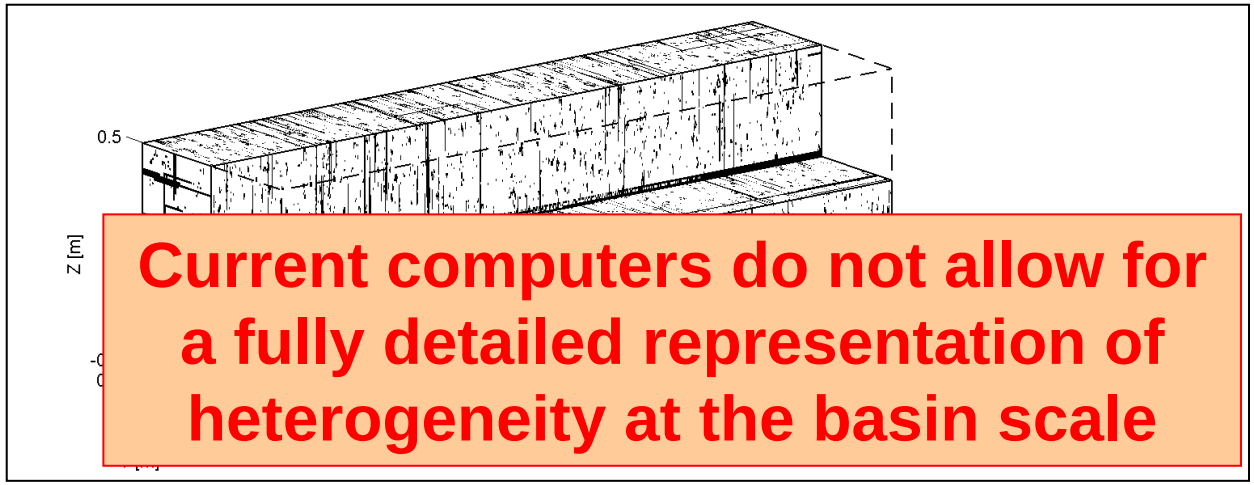

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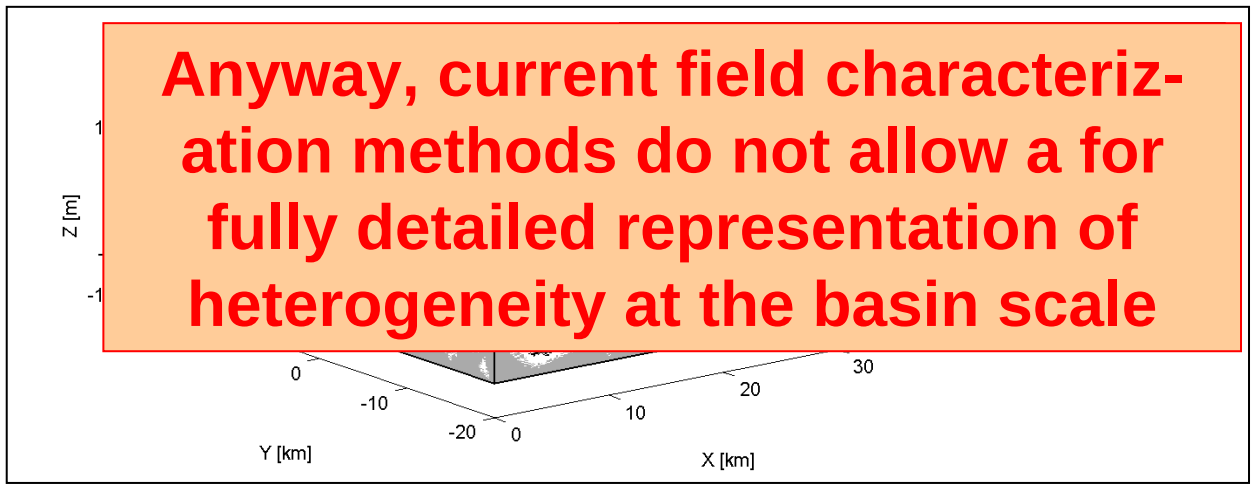


Anyway, current field characterization methods do not allow a for fully detailed representation of heterogeneity at the basin scale

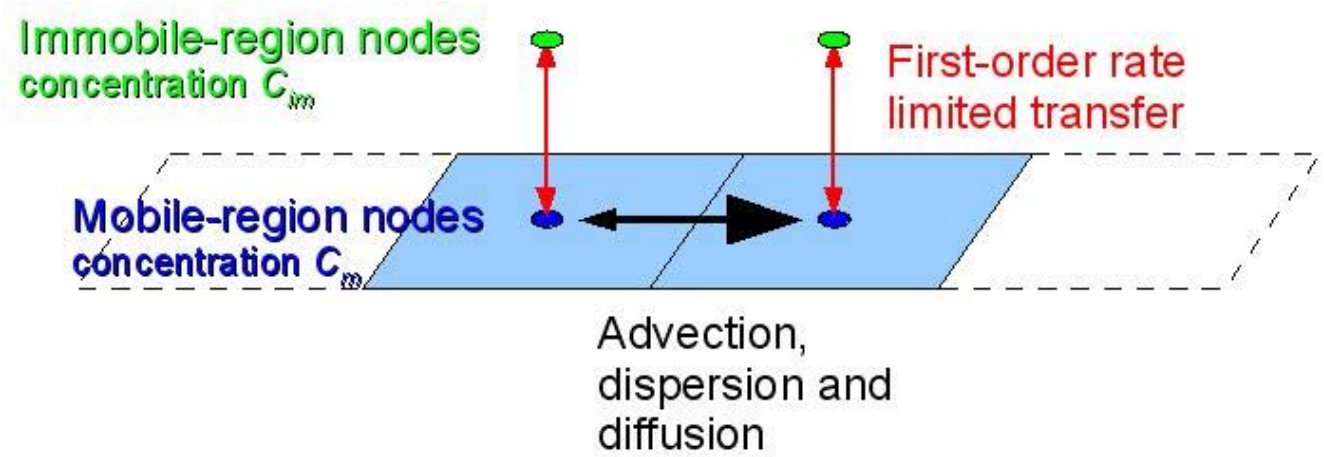
Our approach : FEHM and the GDPM capability

A finite element heat and mass transport code

- Control-volume finite-element formulation
  - More stable than the traditional FE method
  - Equivalent to block-centered FD for orthogonal grids
- Structured and unstructured grids
- Coupled heat and multiphase mass transport
- Reactive solute transport
  - Advection-dispersion equation
  - Dual-porosity formulation : the GDPM capability

Our approach : FEHM and the GDPM capability
The generalized dual-porosity model (1)

- Dual-porosity solute transport model
- Classical dual-porosity models :



- Approximate model for transverse diffusive transfer between rock fractures and matrix

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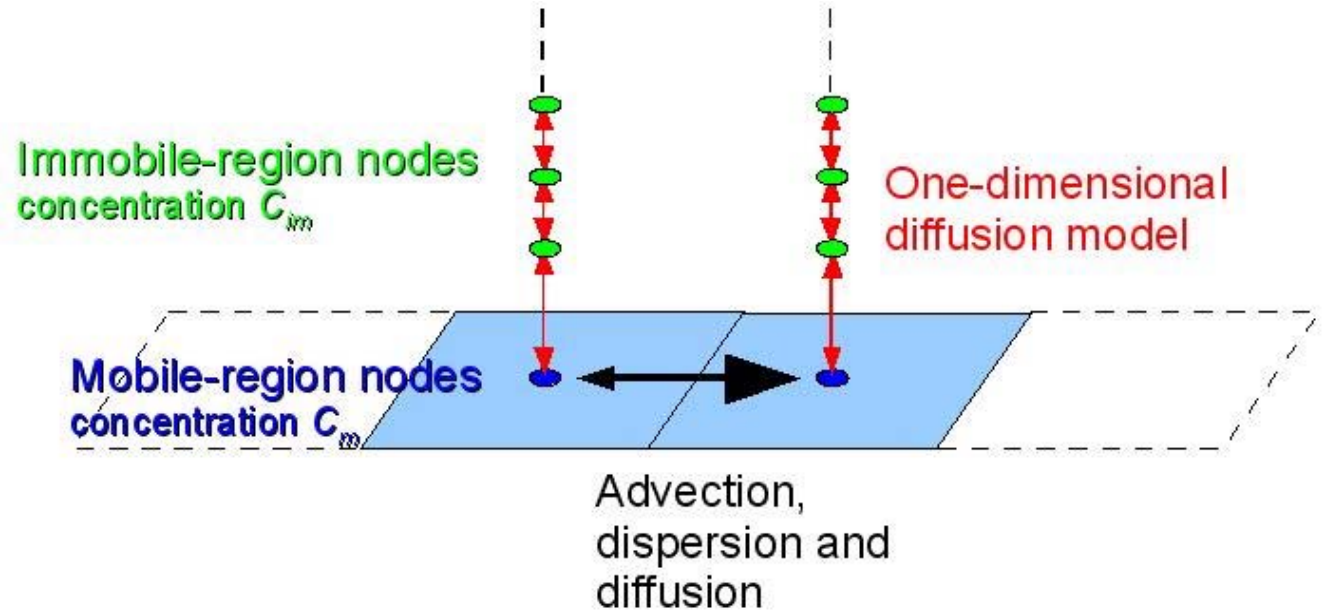
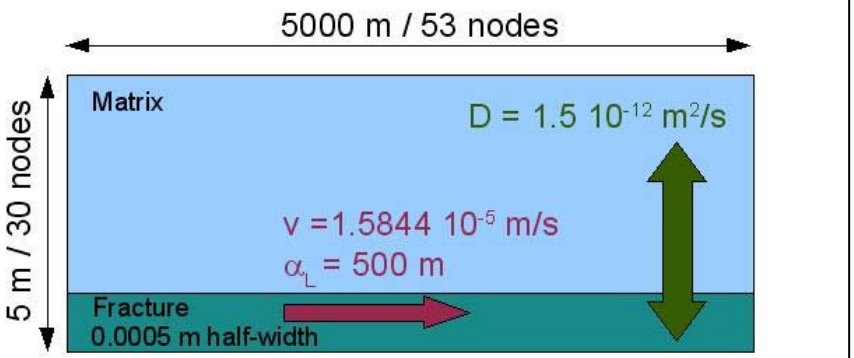
- The generalized dual-porosity model :



- Exact model for transverse diffusive transfer between rock fractures and matrix

Our approach : FEHM and the GDPM capability
The generalized dual-porosity model (3)

- Example : solute transport through a single fracture



Steady-state saturated flow conditions

Step injection at domain inlet at time t=0

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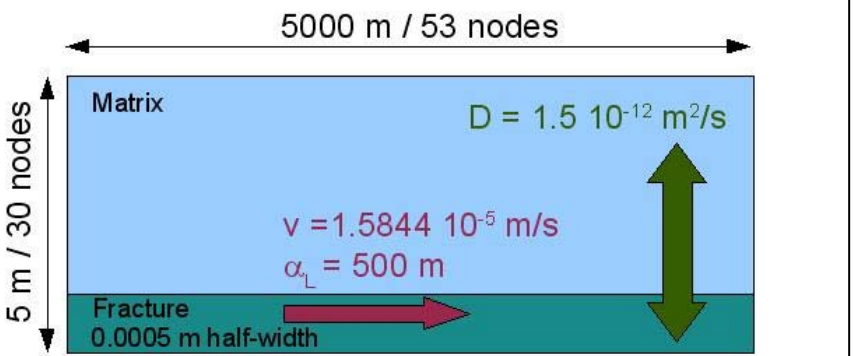

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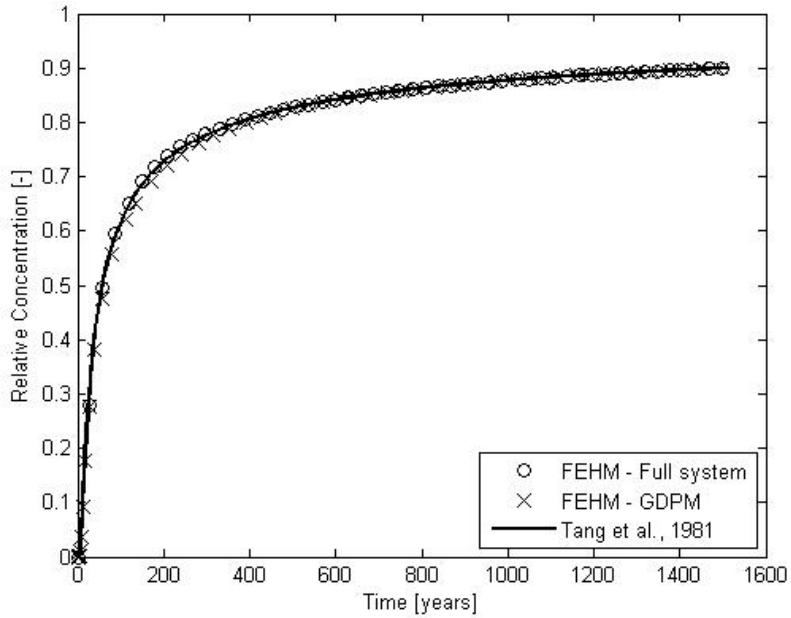

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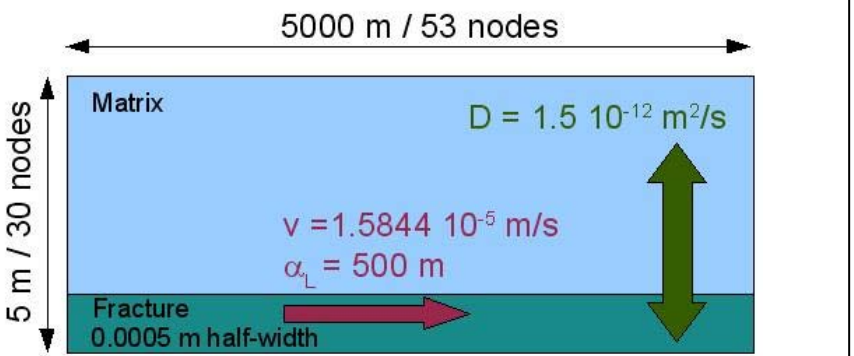

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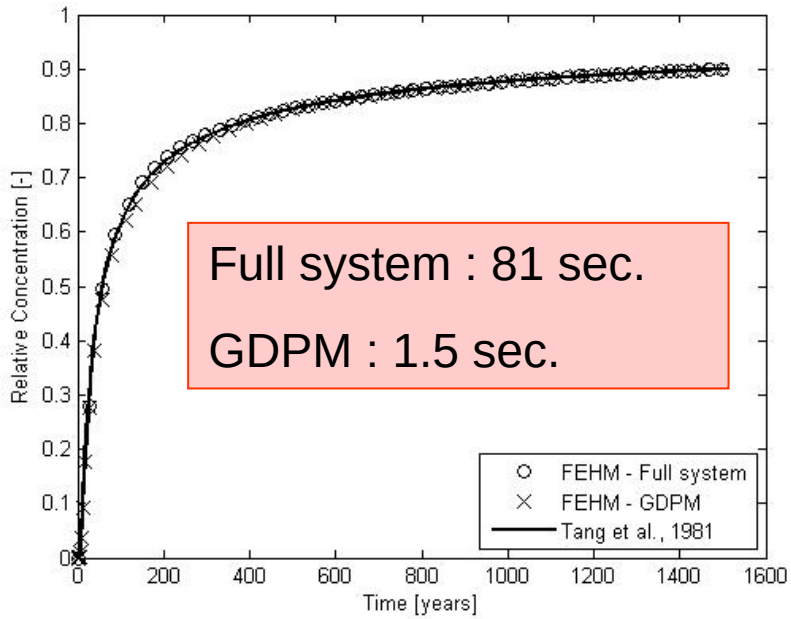

Full system : 81 sec.

GDPM : 1.5 sec.

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- Upscaling methods for flow and solute transport
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- Characterizing heterogeneity in the Piceance basin
  - Markov Chain transition probabilities
  - Example : the Uinta Formation
  - 2D and 3D realizations of heterogeneous blocks of soil
- Preliminary results : the Mahogany zone
- Future work

Characterizing heterogeneity in the Piceance basin
Markov Chain transition probabilities

- Finite number of categorical variables (facies)
- Development of transition probabilities based on core data

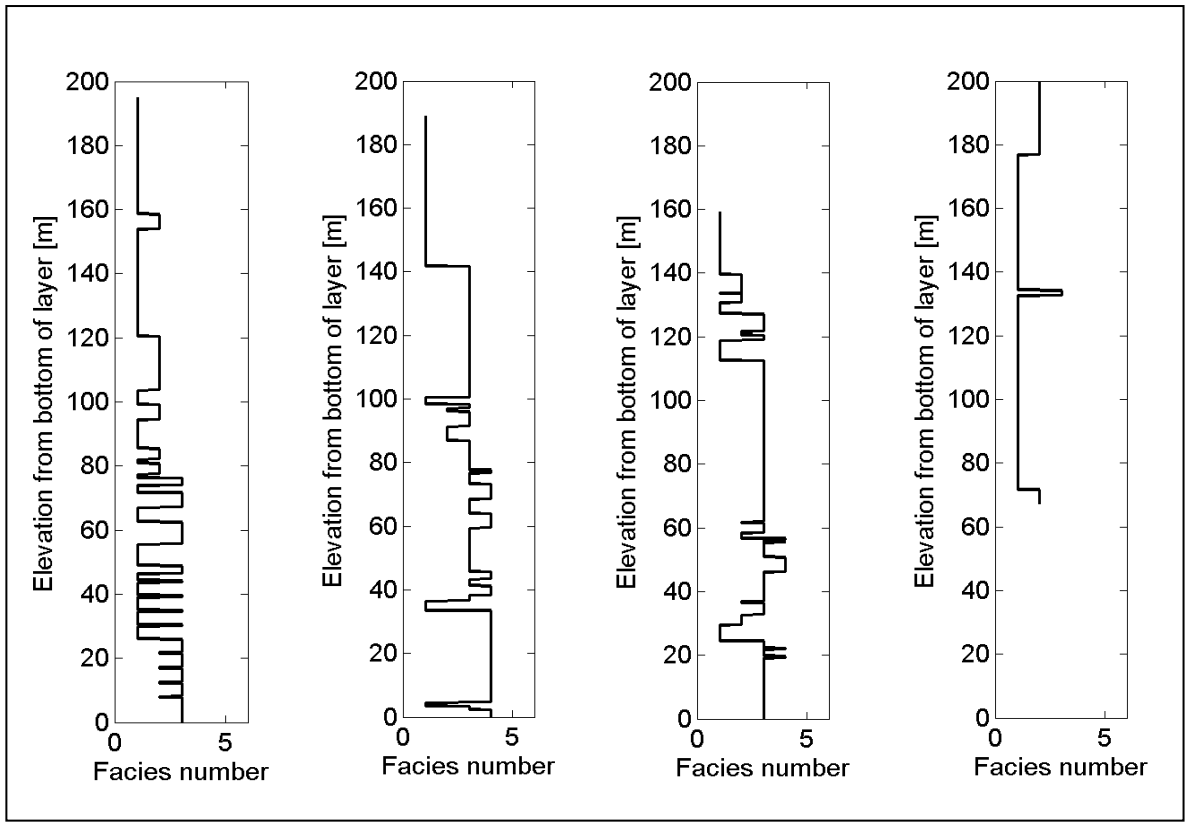
$t_{ij}(h) =$ probability of finding facies *j* at a distance *h* of a location where facies *i* is observed

- Markov Chain model features :
  - Volumetric proportions of facies
  - Mean length of facies
  - Juxtapositional tendencies

Characterizing heterogeneity in the Piceance basin
Example : the Uinta Formation

- Examples of facies transitions based on available core data :

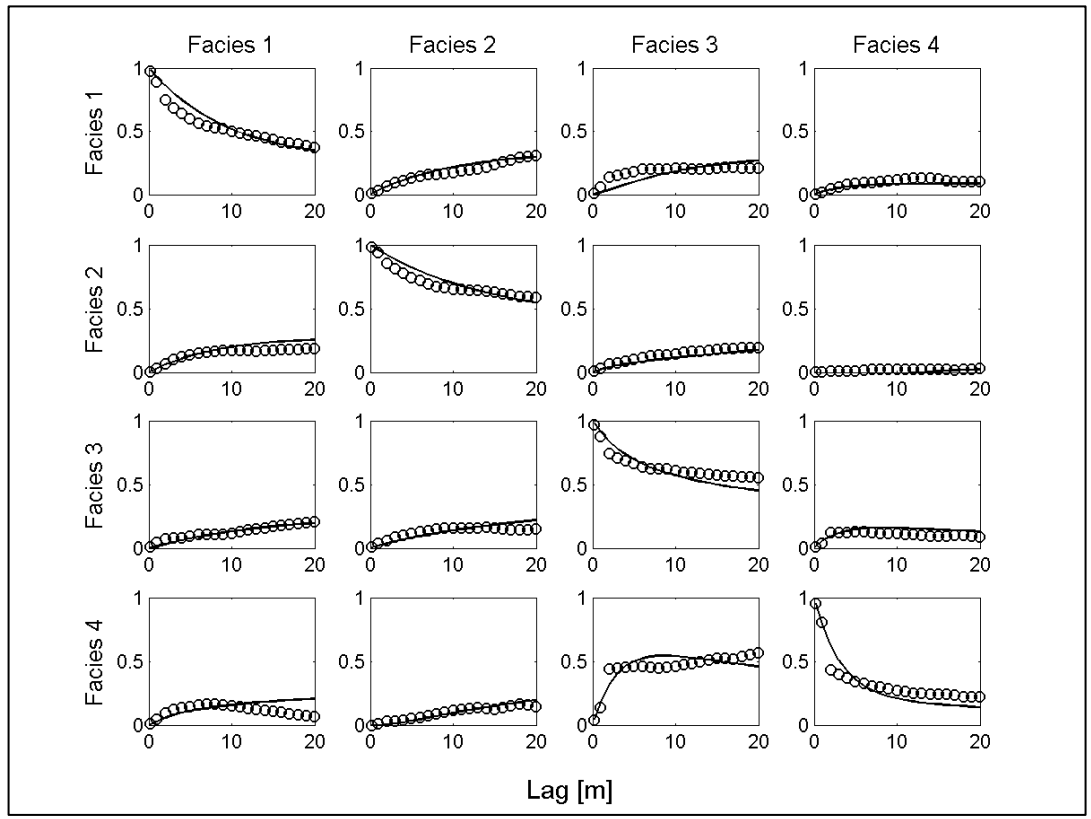
4 facies :
1 : siltstone
2 : sandstone
3 : marlstone
4 : oil shale



Characterizing heterogeneity in the Piceance basin
Example : the Uinta Formation (2)

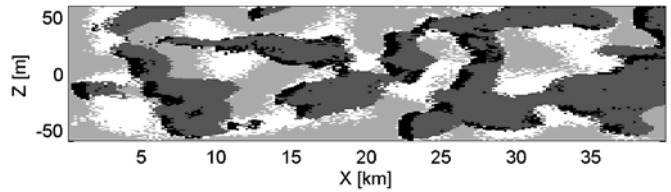
- Vertical transition probability model :

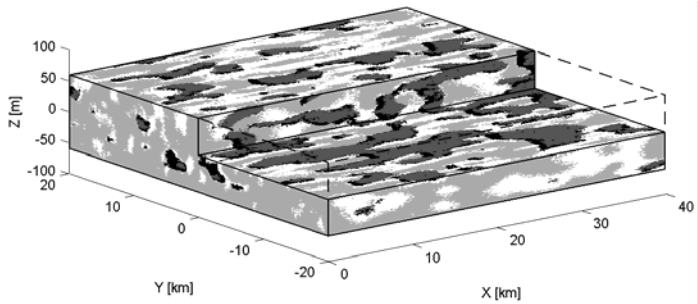
Legend :
o : experimental TP
– : Markov Chain model



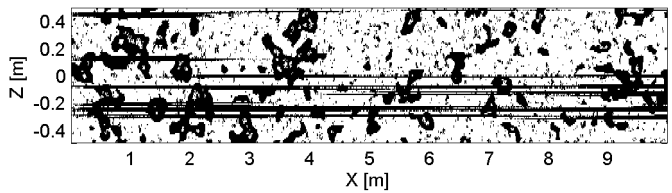
Characterizing heterogeneity in the Piceance basin

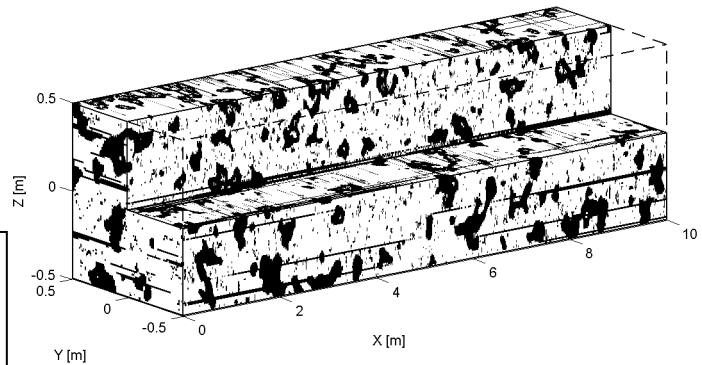
2D and 3D realizations of heterogeneous blocks of soil





Uinta Formation





Leached Zone :

Model of fracture distribution Nahcolite dissolution

Preliminary results : the Mahogany zone
Model of heterogeneity

- Models of fracture distribution resulting from hydraulic fracturing
- Two-dimensional transition probability model
  - Volumetric proportion of fractures : 20 %
  - Mean length of horizontal fractures : 5 m
  - Mean thickness of horizontal fractures : 2 cm
  - Mean length of vertical fractures : 20 cm
  - Mean thickness of vertical fractures : 1 cm

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Model of heterogeneity

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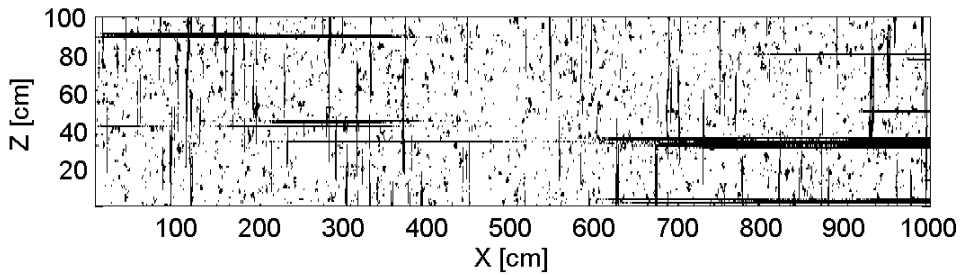
Random realization



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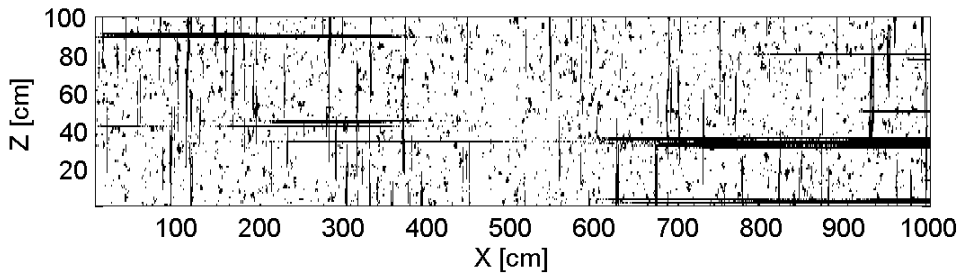
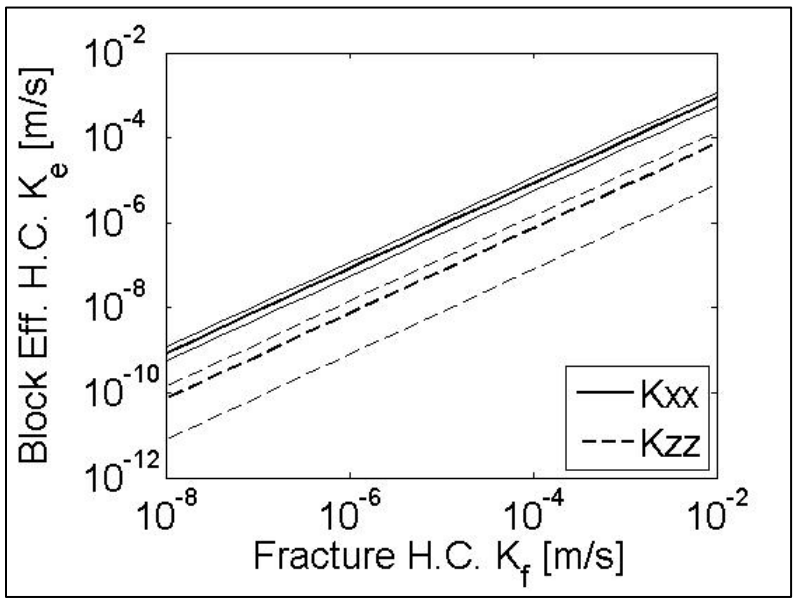


- Two-dimensional simulations of flow and transport
  - 5 m x 1 m blocks
  - 1 cm x 1 cm cells (5,000,000 cells)
  - 20 real. (flow) and 10 real. (transp.)

Preliminary results : the Mahogany zone
Upscaling of flow

- Matrix sat. hydraulic conductivity : 10^{-14} m/s
- Fracture sat. hydraulic conductivity : 10^{-2} – 10^{-8} m/s



Linear dependence !

$$K_e = \theta_f K_f$$

Hor. Flow : $\theta_f = 0.083$

Vert. Flow : $\theta_f = 0.0075$

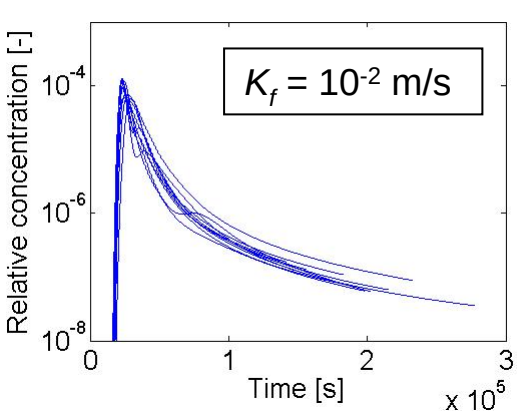
Horizontal flow

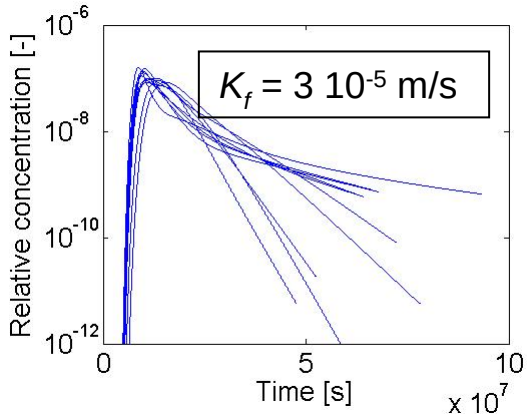
High connectivity →

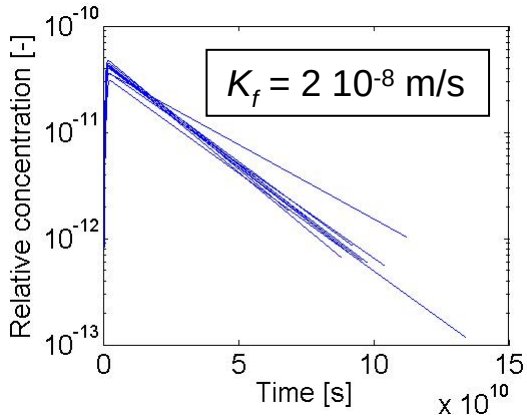
perfectly stratified model, with θ_f ~ volume proportion of horizontal fractures

Preliminary results : the Mahogany zone
Upscaling of solute transport

- Results for 10 realizations







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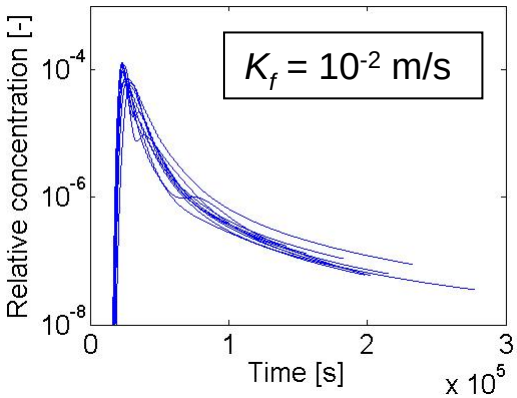

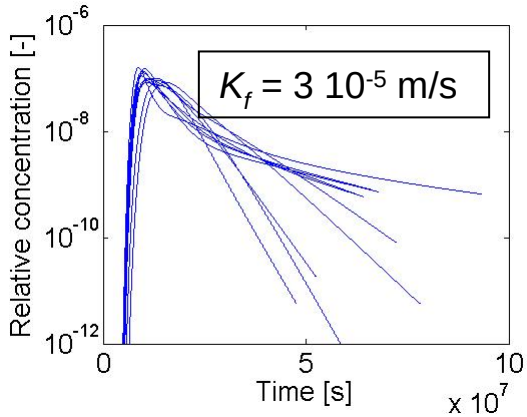

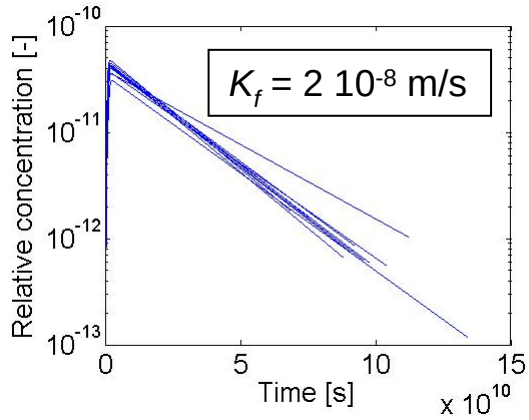

High K_f

Transport governed by connected paths properties

Preliminary results : the Mahogany zone
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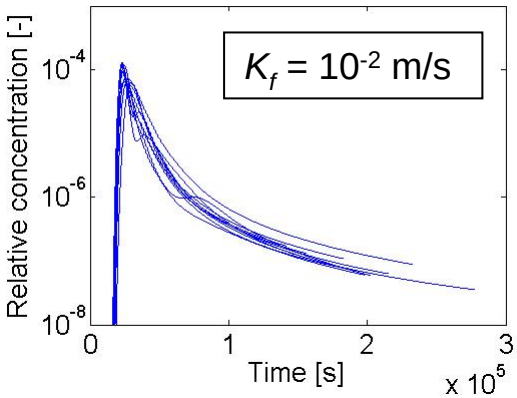

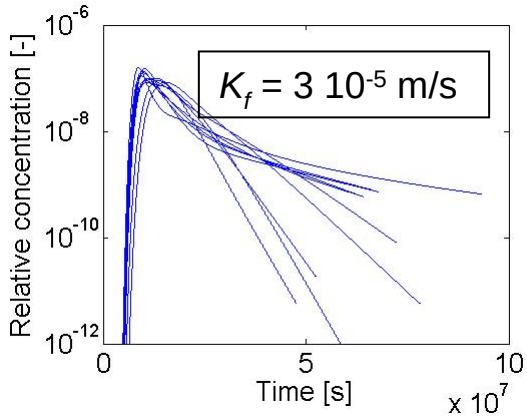

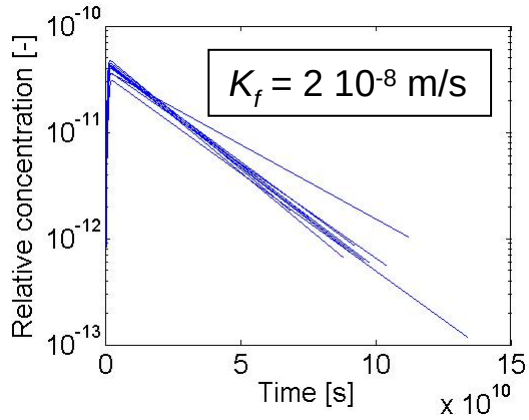

High K_f

Transport governed by connected paths properties

Intermediate K_f

The potential presence of less connected paths (i.e. through vertical fractures) dominates late-time BTC features

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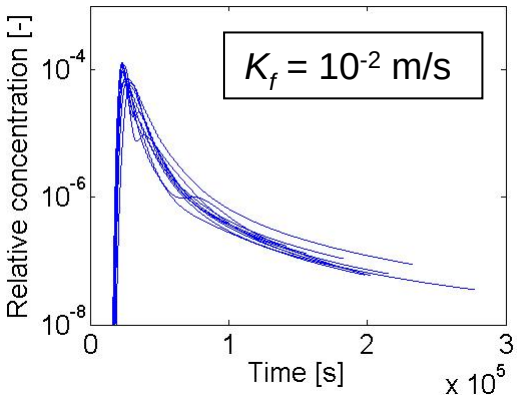

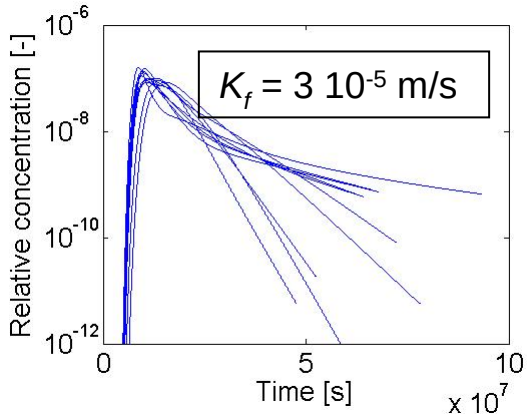

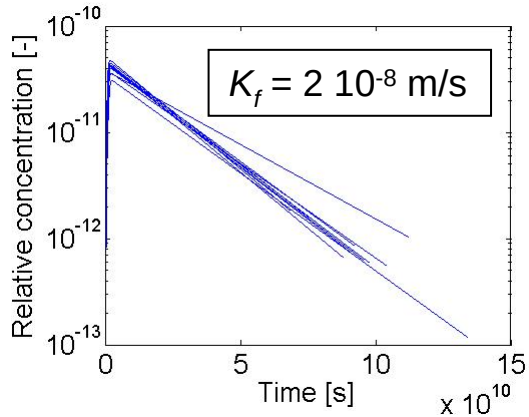

High K_f

Transport governed by connected paths properties

Intermediate K_f

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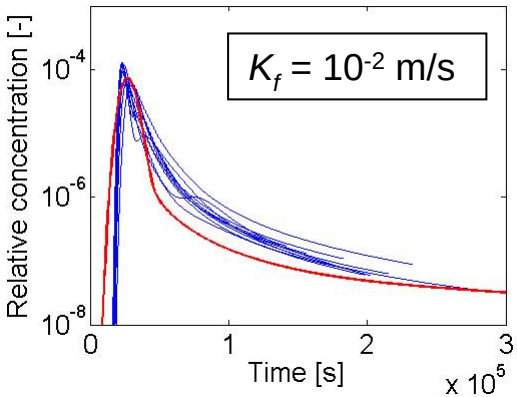
Low K_f

Transport governed by diffusion through large matrix blocks

Preliminary results : the Mahogany zone
Upscaling of solute transport (3)

- GDPM results – perfectly stratified assumption



High K_f

Small effect of diffusion, advection through the largest fracture

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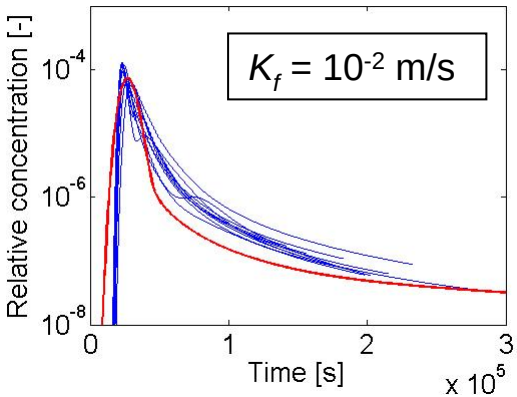

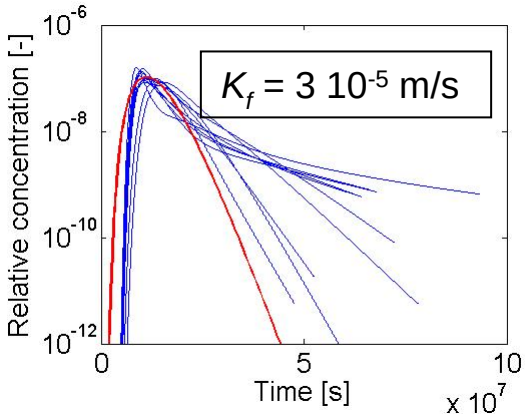

High K_f

Small effect of diffusion, advection through the largest fracture

Intermediate K_f

Advection-dominated transport and poor performances of the GDPM

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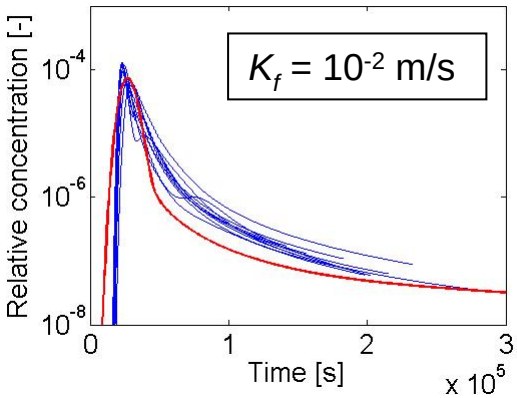
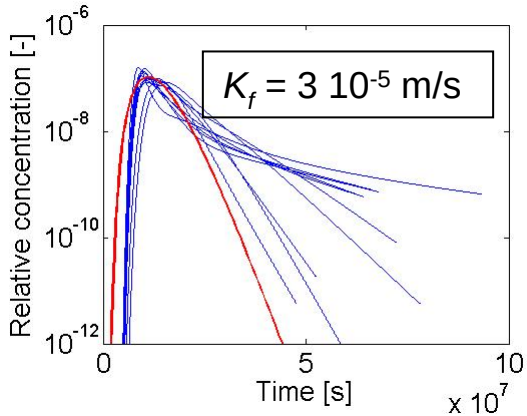
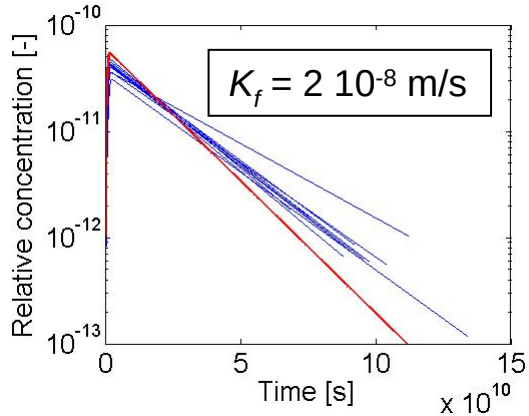
Upscaling of solute transport (3)

- GDPM results – perfectly stratified assumption







High K_f

Small effect of diffusion, advection through the largest fracture

Intermediate K_f

Advection-dominated transport and poor performances of the GDPM

Low K_f

Matrix diffusion-dominated transport – good performances of the GDPM

Future work

- Determination of effective GDPM parameters
- Sensitivity analysis for flow and transport
  - In fractured media
    - Volumetric proportion of fractures
    - Mean length of fractures vs block size
    - Hydraulic conductivity of fractures
    - Dimensionality (2D vs 3D simulations)
  - In heterogeneous porous media
    - Horizontal TP model
    - Facies hydraulic conductivity
- Heat transport
- Coupled heat and solute transport

- Thank you for your attention !
- Any questions or comments ?