The reactive transport benchmark : A reference solution for 1D easy level ?

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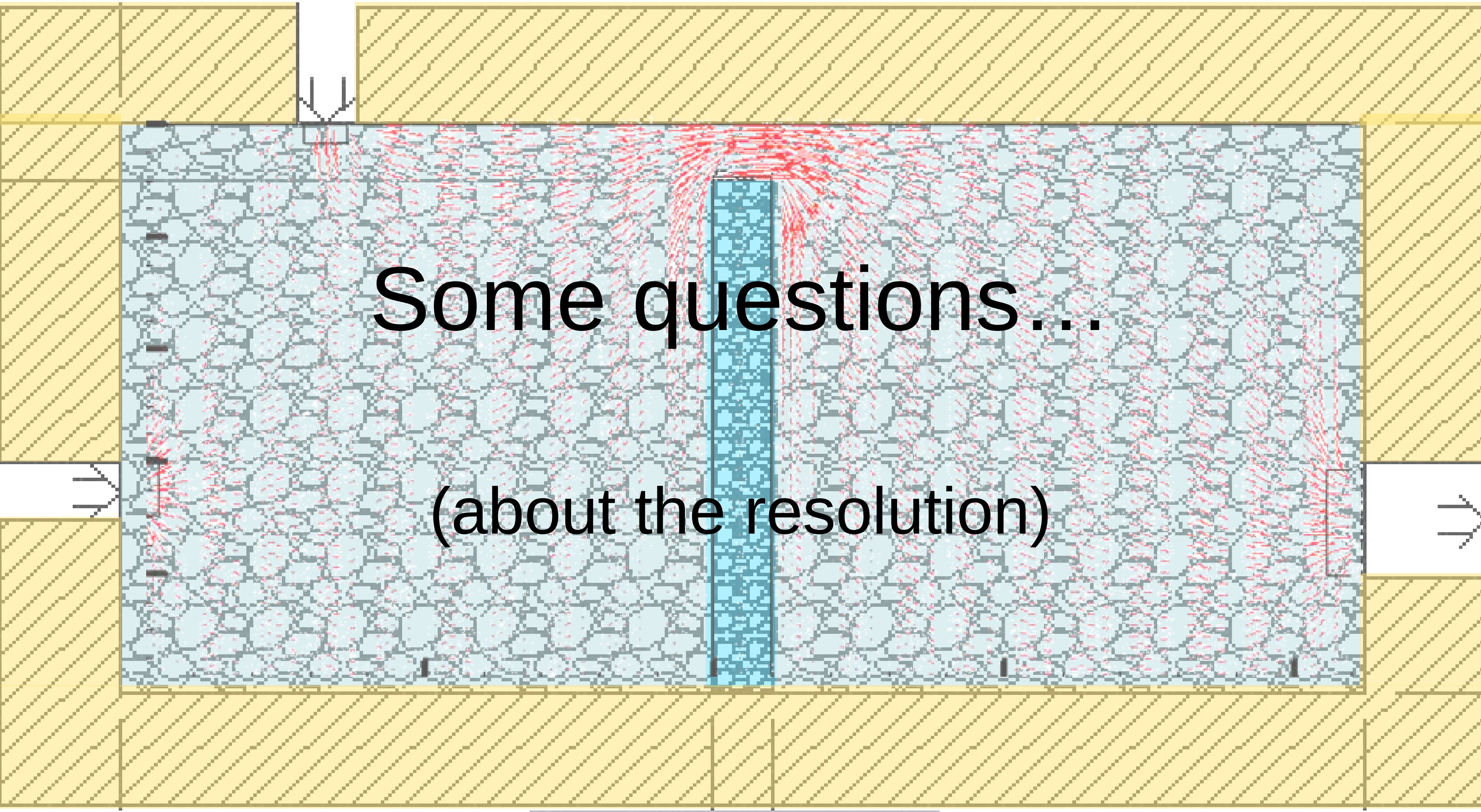
Outline

- **Introduction: objectives of the benchmark**
- **The 1D easy level**
- **Some results**



Some questions…

(about the resolution)

Operator Splitting / Global Approach

Operator Splitting:

- Iterative – Non iterative
- OS scheme
- OS errors

Global Approach:

- Scheme : DSA / DAE
- Resolution of non linear system
- CPU time / Memory

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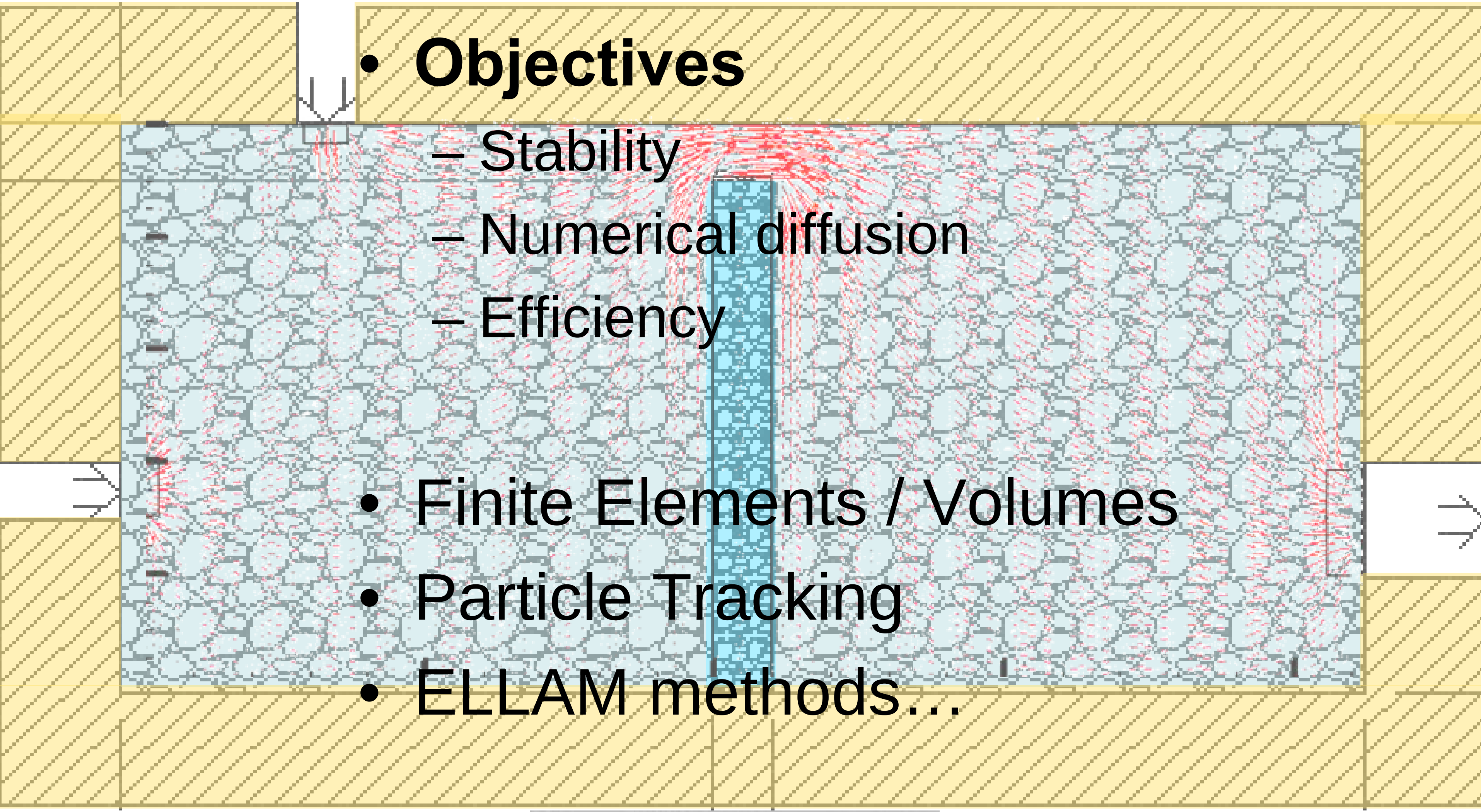
Space discretisation



- **Objectives**
  - Stability
  - Numerical diffusion
  - Efficiency

- Finite Elements / Volumes
- Particle Tracking
- ELLAM methods…

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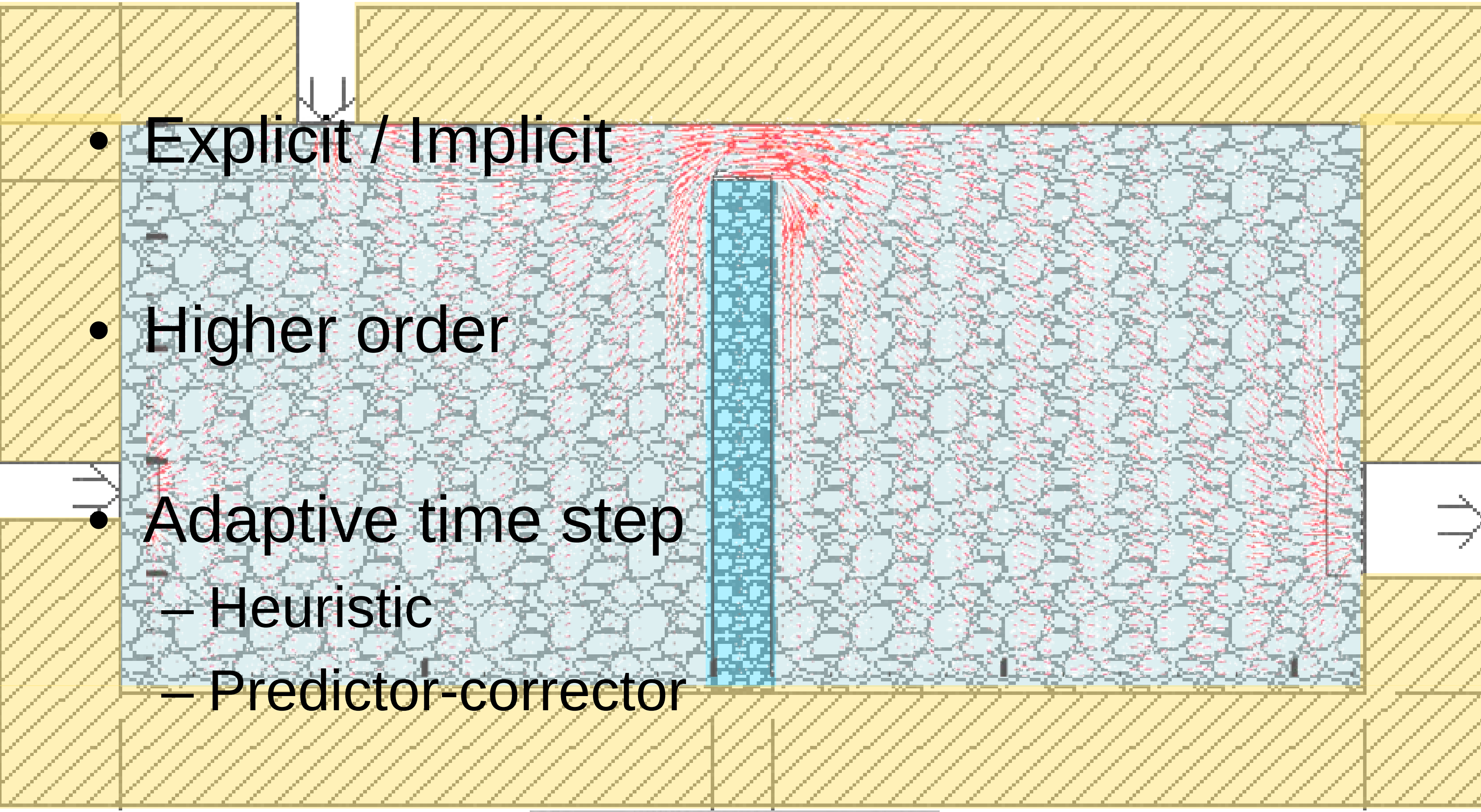
Time discretisation



- Explicit / Implicit
- Higher order
- Adaptive time step
  - Heuristic
  - Predictor-corrector

About convergence…

- Iterative method for chemistry
- Iterative method for transport (SIA)
- Iterative method for global approach
- What about very small concentration
  - From transport $C = 10^{-300}$…
  - Numerical problem if $C = 0$

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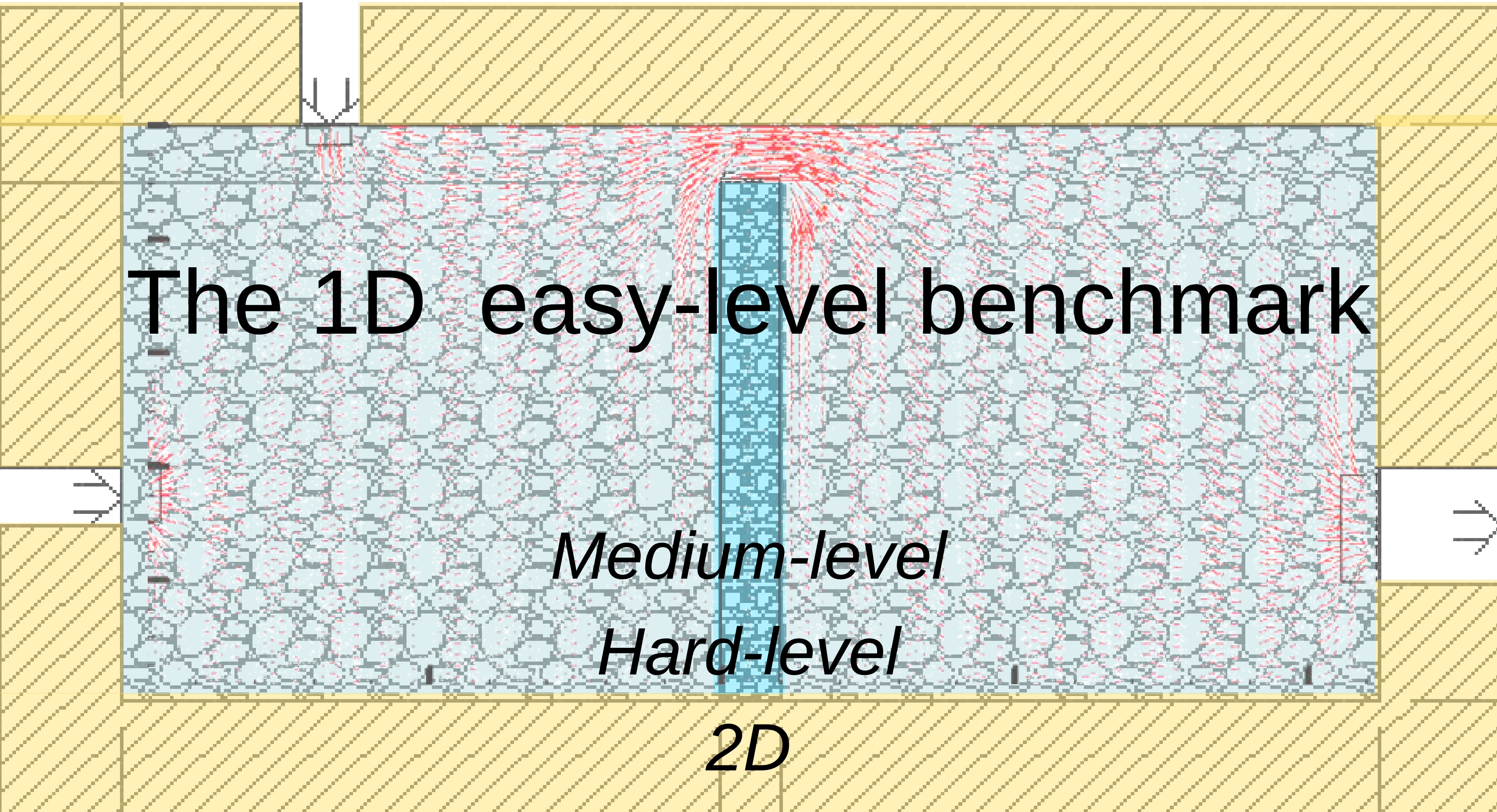


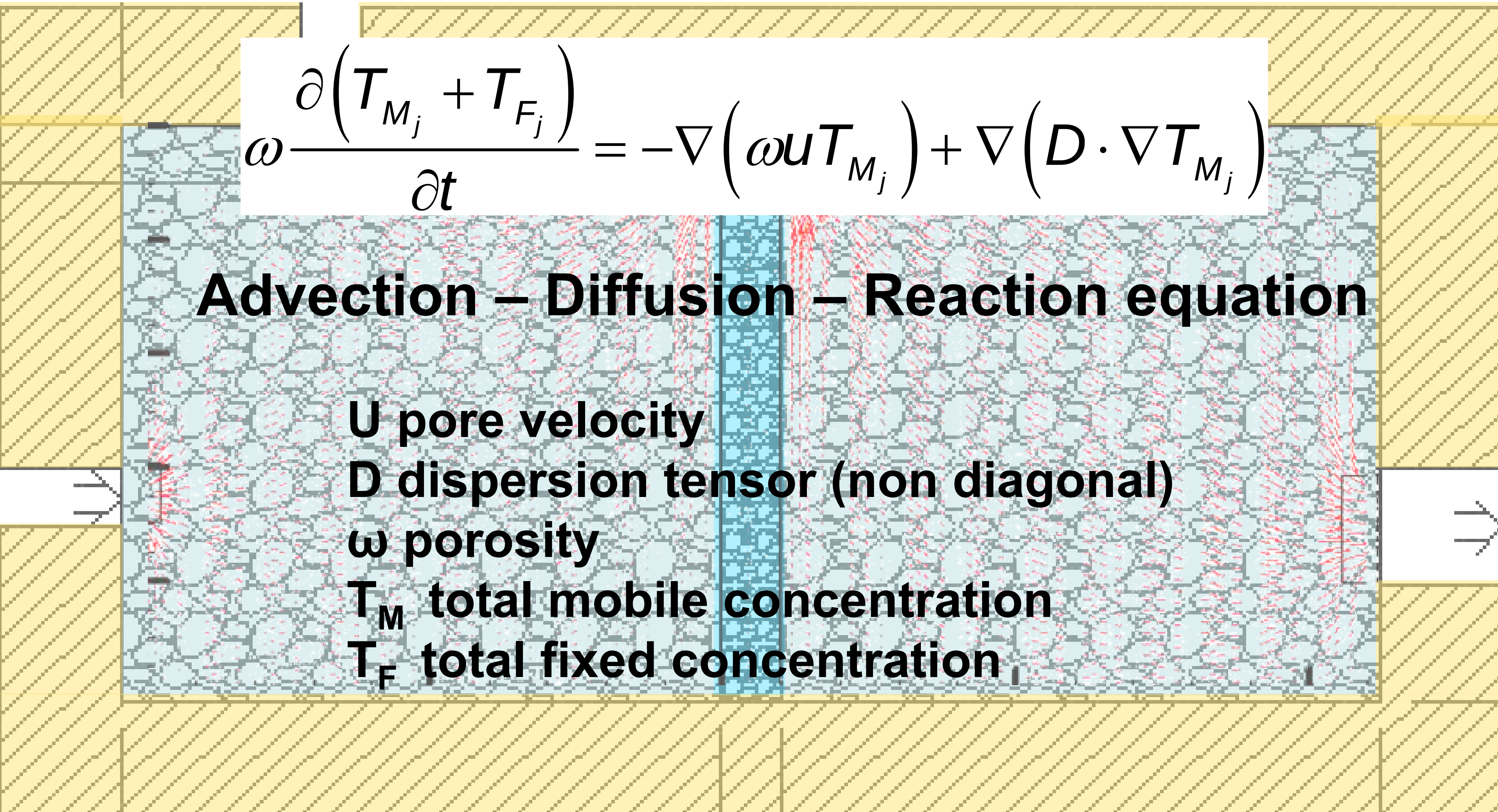
The 1D easy-level benchmark

Medium-level

Hard-level

2D

Reactive transport modelling



$$\omega \frac{\partial \left(T_{M_j} + T_{F_j} \right)}{\partial t} = -\nabla \left(\omega u T_{M_j} \right) + \nabla \left(D \cdot \nabla T_{M_j} \right)$$

Advection – Diffusion – Reaction equation

U pore velocity
D dispersion tensor (non diagonal)
ω porosity
T_M total mobile concentration
T_F total fixed concentration

Equilibrium chemistry

Mobile Species | **Non mobile Species**

Reactions

$$\sum_{j=1}^{NxM} a_{i,j} X_j \rightleftarrows C_i$$

$$\sum_{j=1}^{NxM} as_{i,j} X_j + as_{i,s} S \rightleftarrows CS_i$$

Mass action laws

$$C_i = K_i \cdot \prod_{j=1}^{NxM} X_j^{a_{i,j}}$$

$$CS_i = Ks_i \cdot \prod_{j=1}^{NxM} X_j^{as_{i,j}} \cdot S^{as_{i,s}}$$

Conservation laws

$$T_j = X_j + \sum_{i=1}^{NcM} a_{i,j} \cdot C_i + \sum_{i=1}^{NcS} as_{i,j} \cdot CS_i$$

$$TS = S + \sum_{i=1}^{NcS} as_{i,s} \cdot CS_i$$

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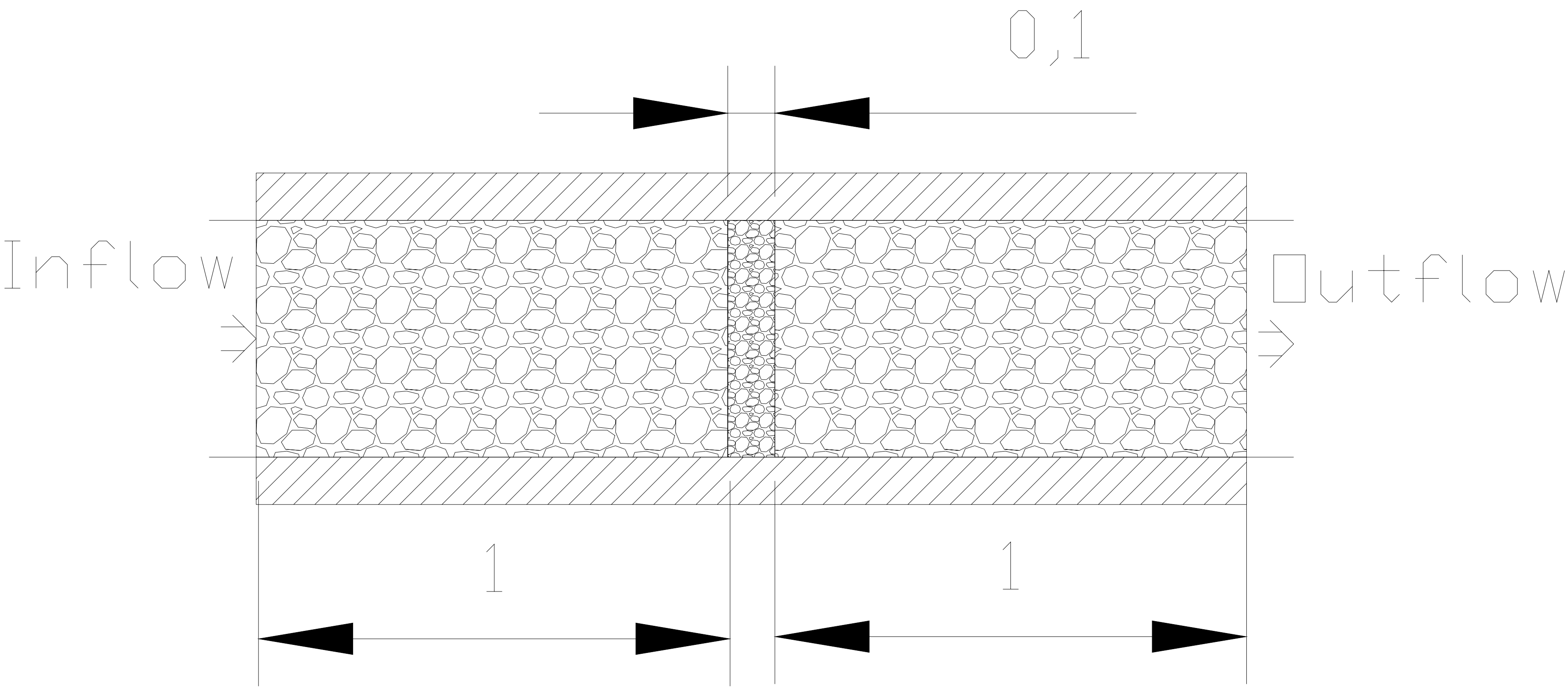
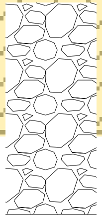
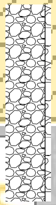
The 1D reactive domain





High permeability
Low porosity
Low reactivity



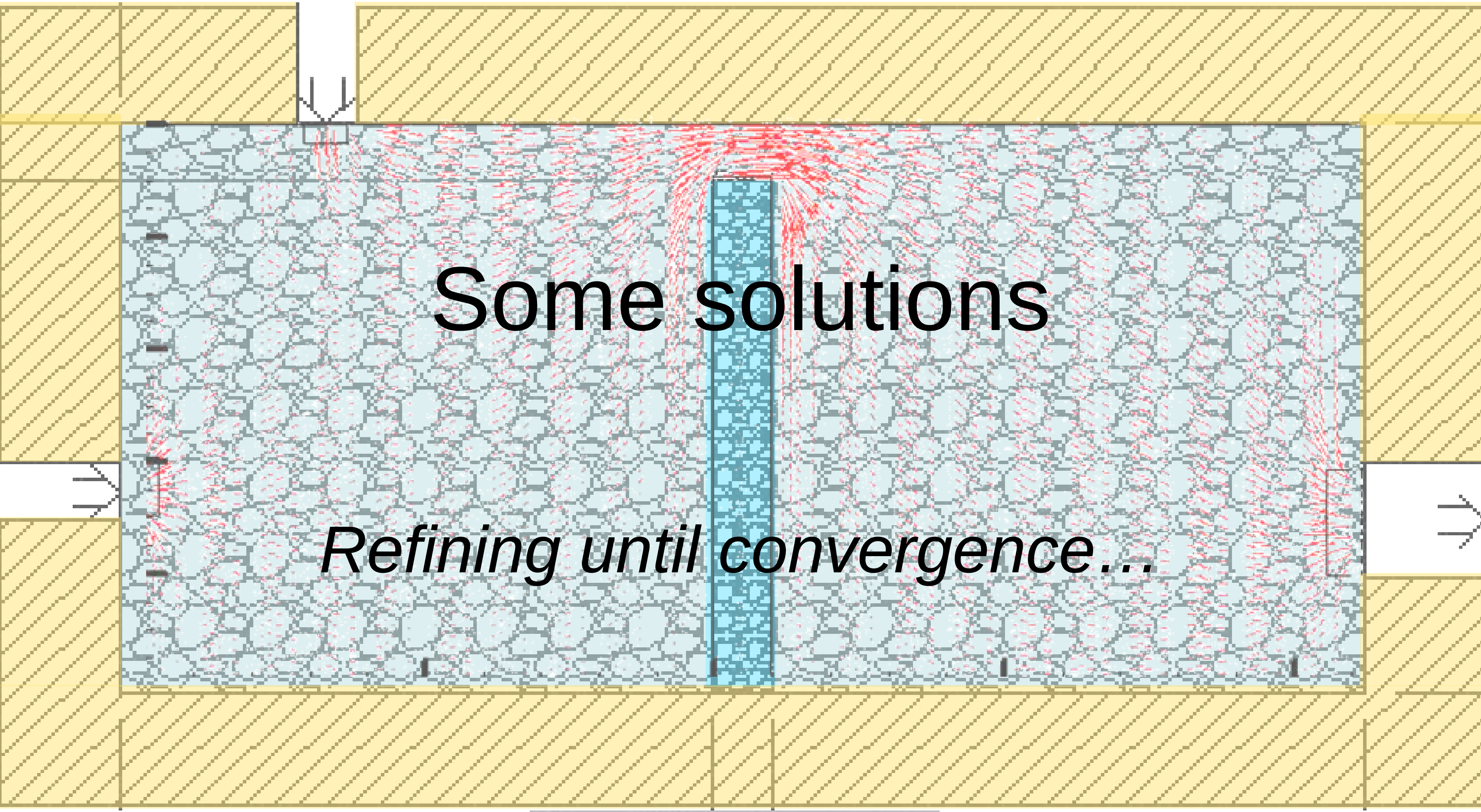
Low permeability
High porosity
High reactivity

Chemical reactions

	X_1	X_2	X_3	X_4	S	K
C_1	0	-1	0	0	0	1.00E-12
C_2	0	1	1	0	0	1
C_3	0	-1	0	1	0	1
C_4	0	-4	1	3	0	0.1
C_5	0	4	3	1	0	1.00E+35
CS_1	0	3	1	0	1	1.00E+6
CS_2	0	-3	0	1	2	1.00E-01
Total ($m.L^{-3}$)	T_1	T_2	T_3	T_4	TS	
Initial for medium A	0	-2	0	2	1	
Initial for medium B	0	-2	0	2	10	

Some solutions

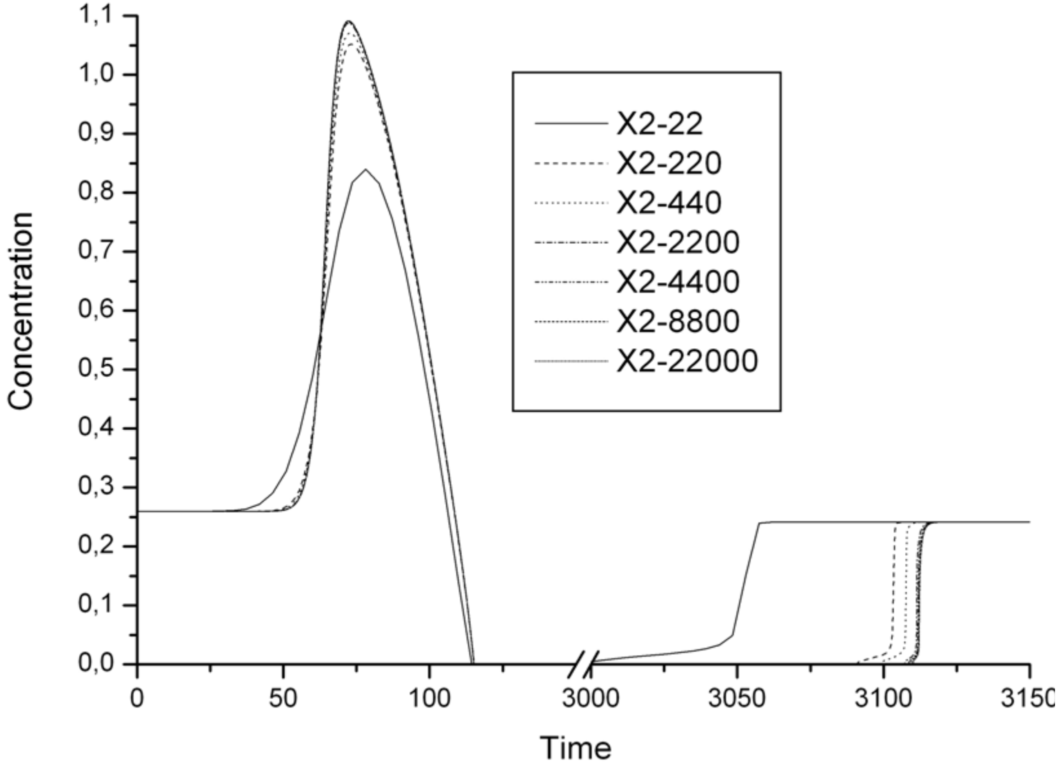
Refining until convergence…

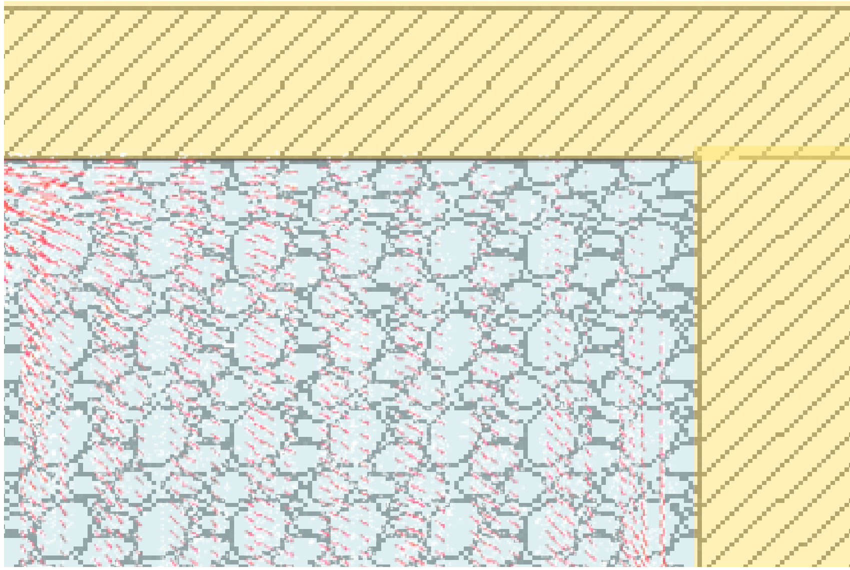


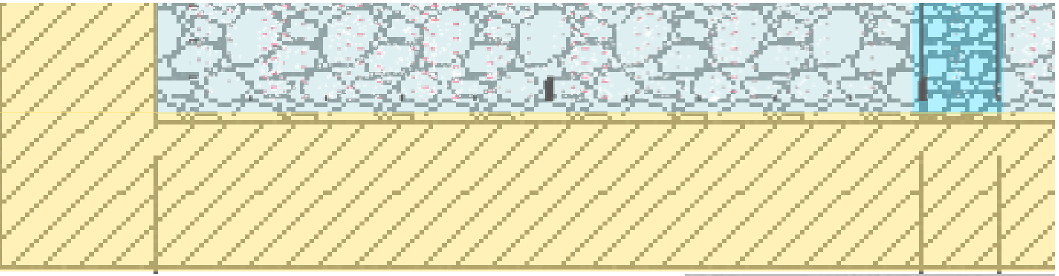
SPECY

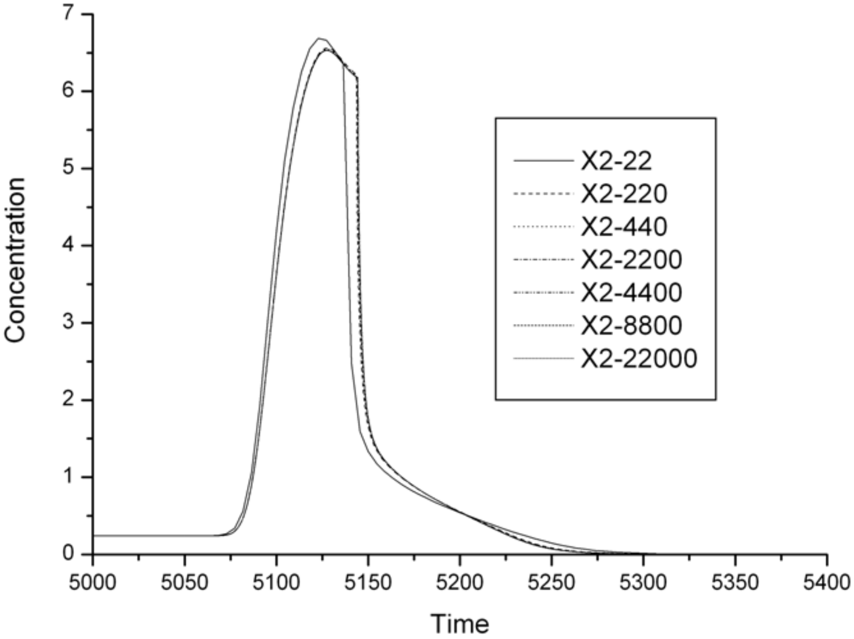
- **SNIA OS scheme**
- **Discontinuous finite element for convection**
  - explicit time step, constant
  - CFL = 1
- **Mixed hybrid finite elements for dispersion**
  - Implicit time step, constant

Elution curves for X2

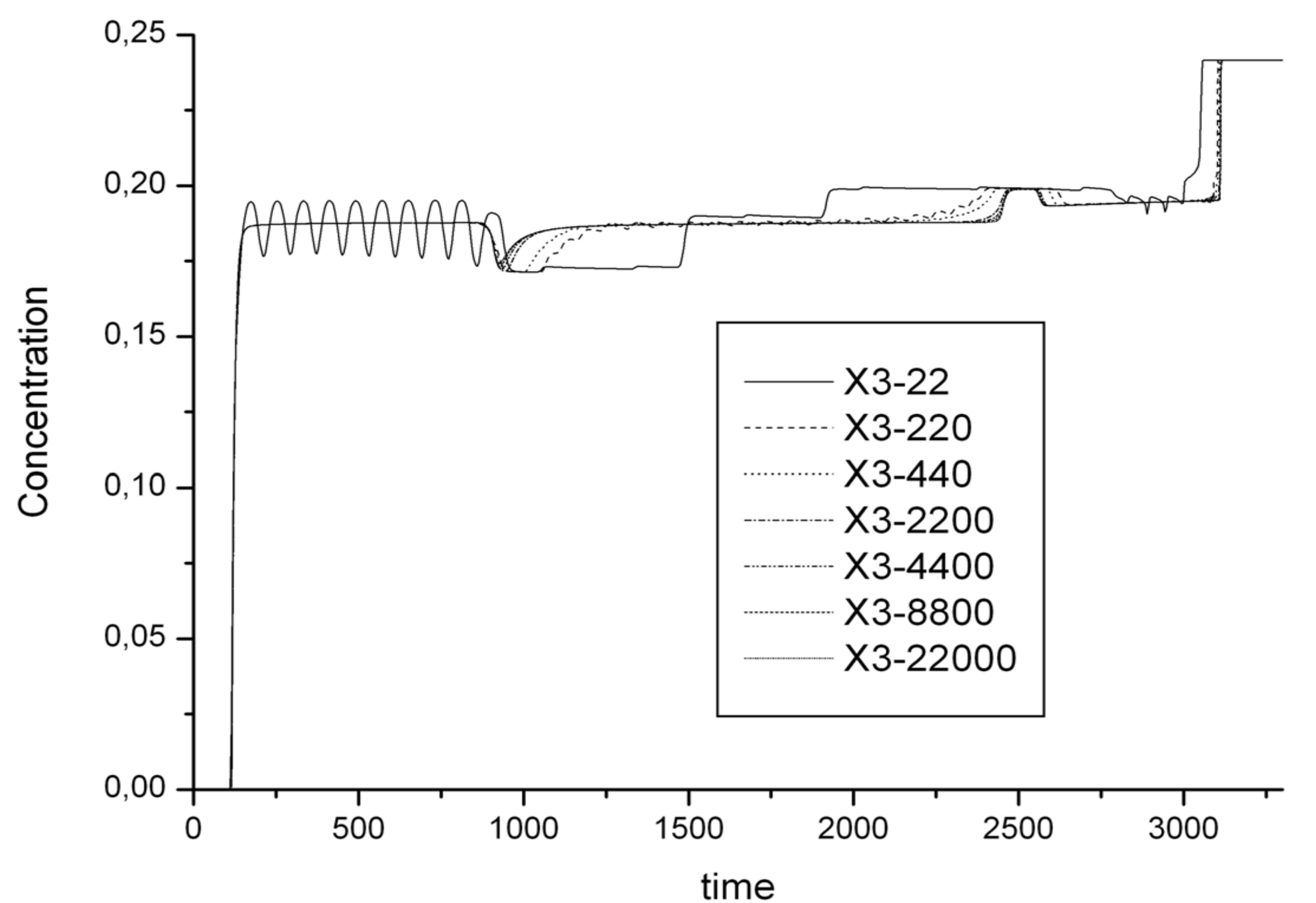




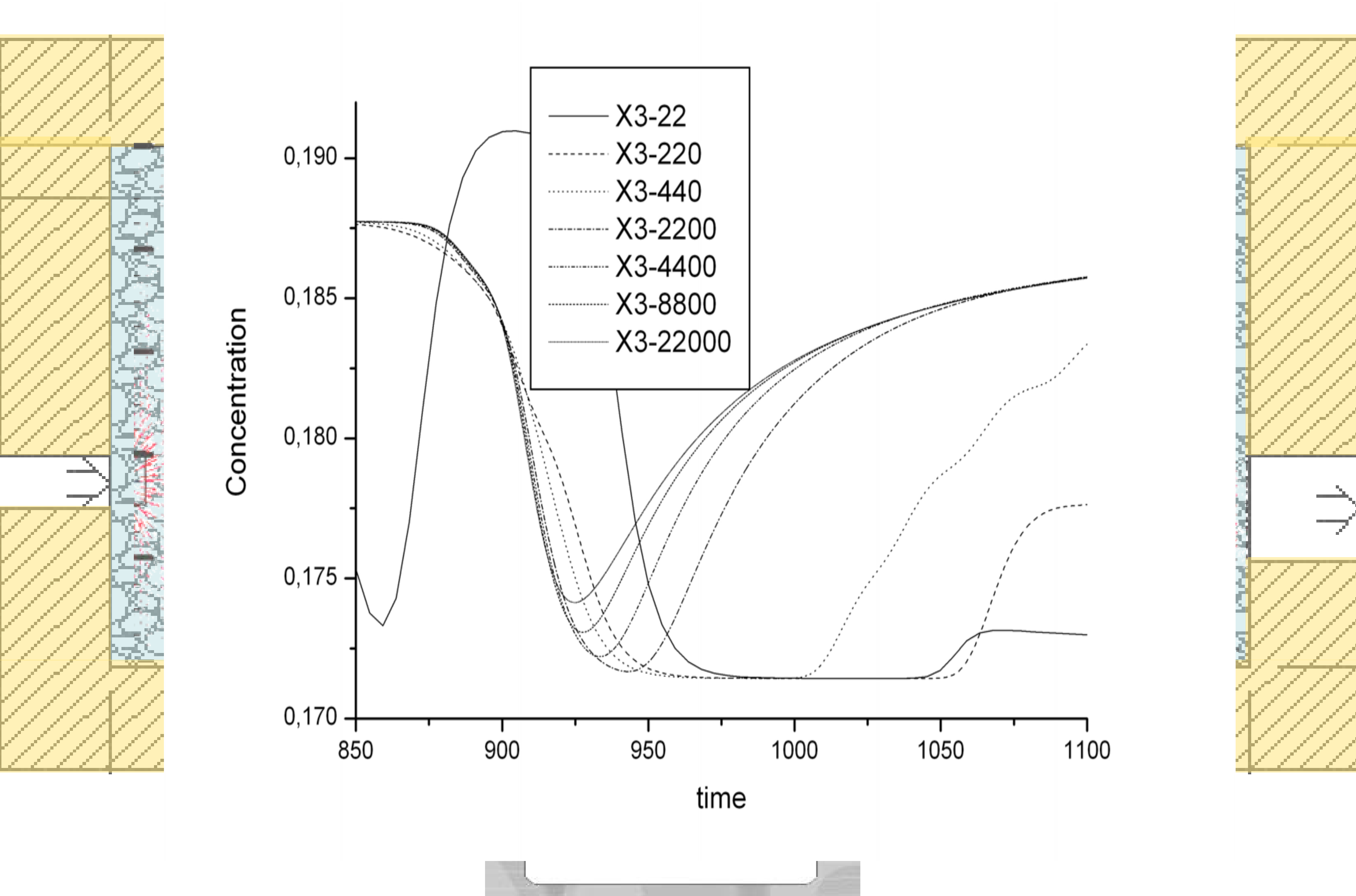




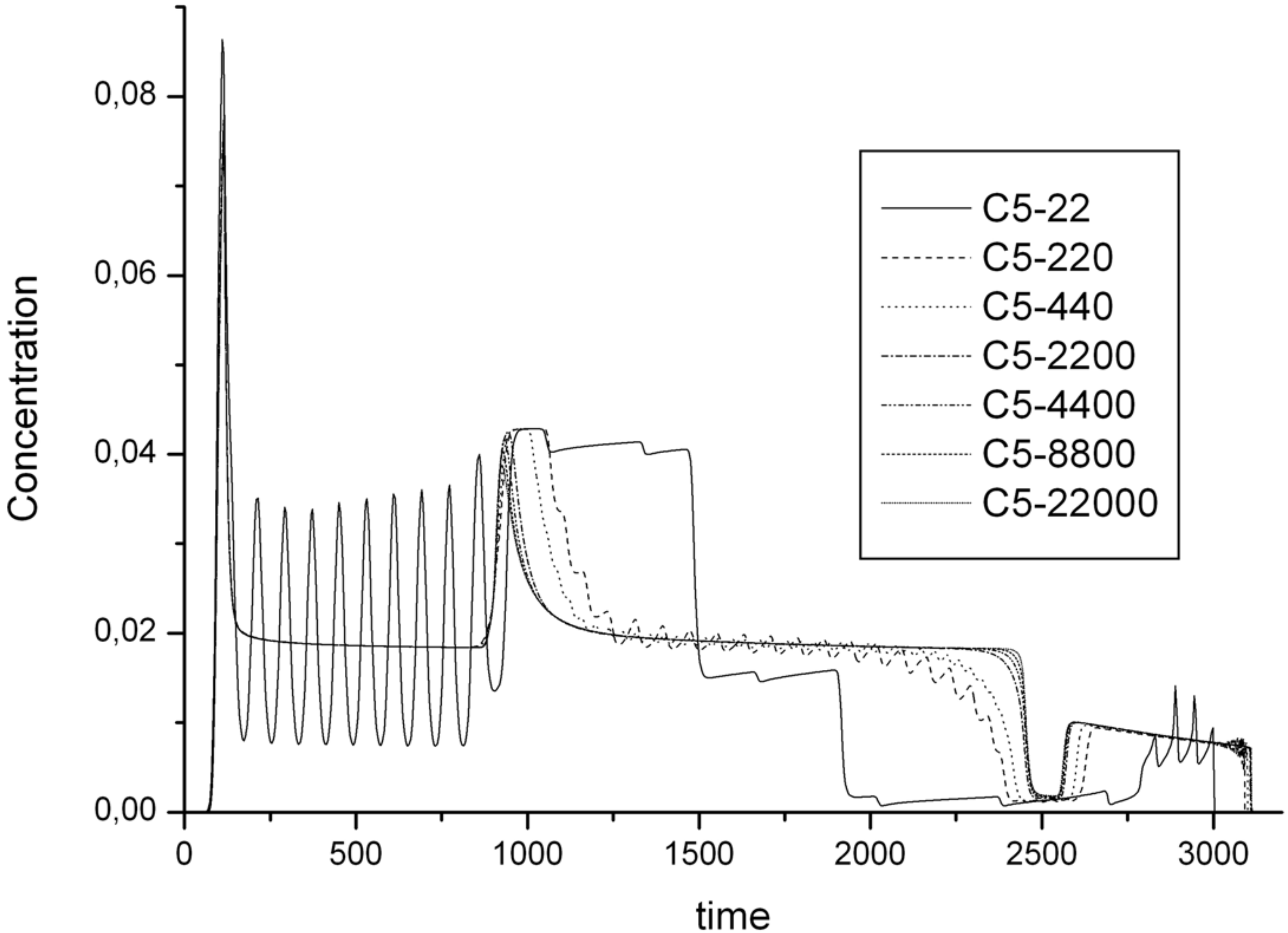
Elution curves for X3



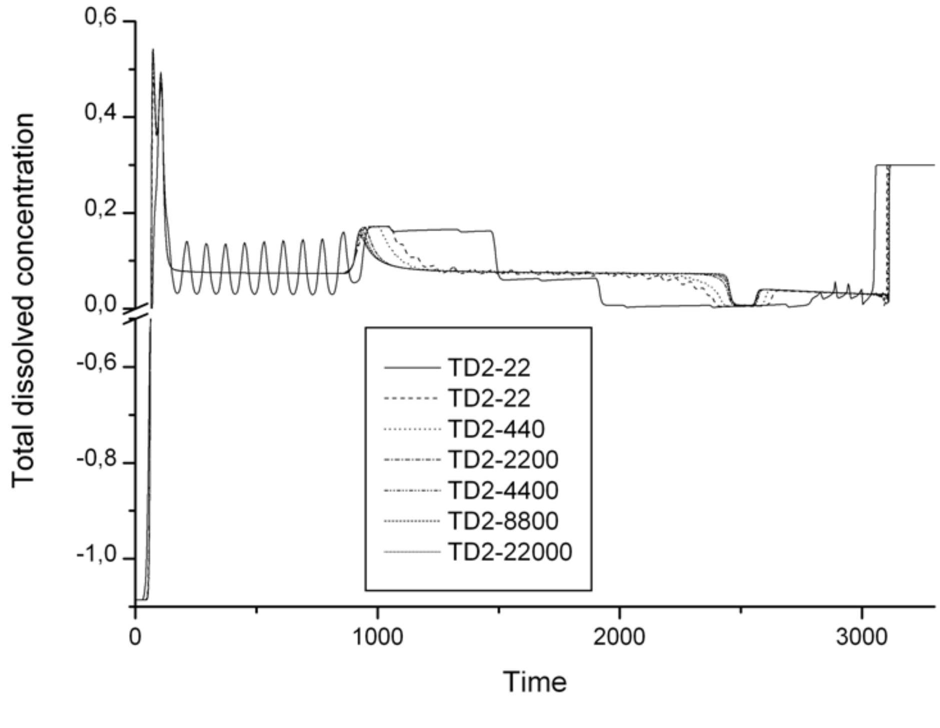
Zoom on elution curves for X3

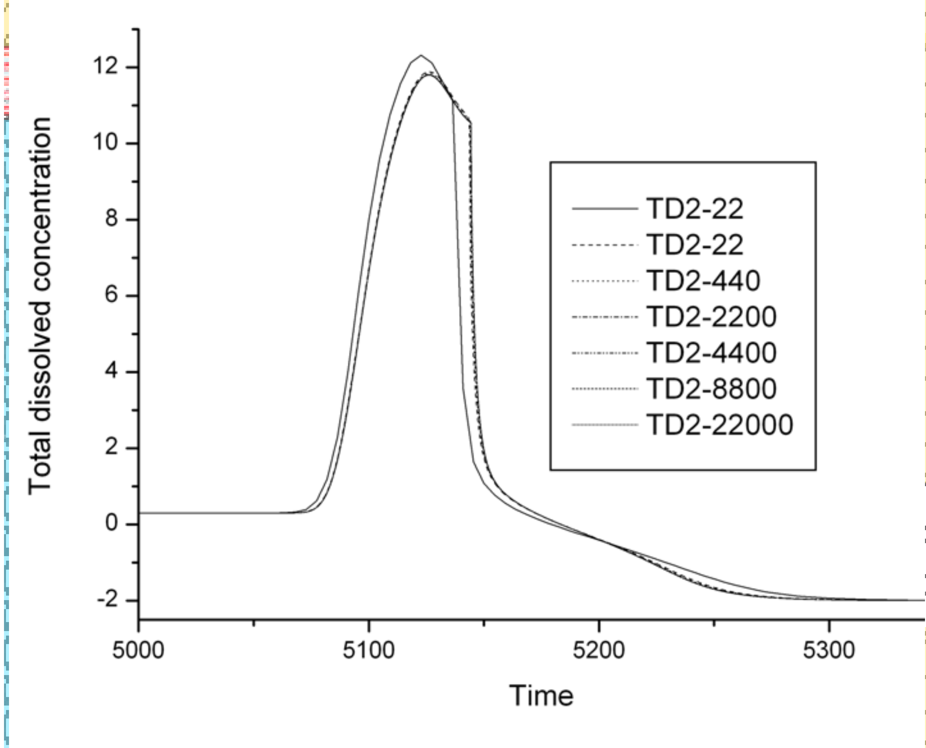


Elution curves for C5



Elution curves for total X2





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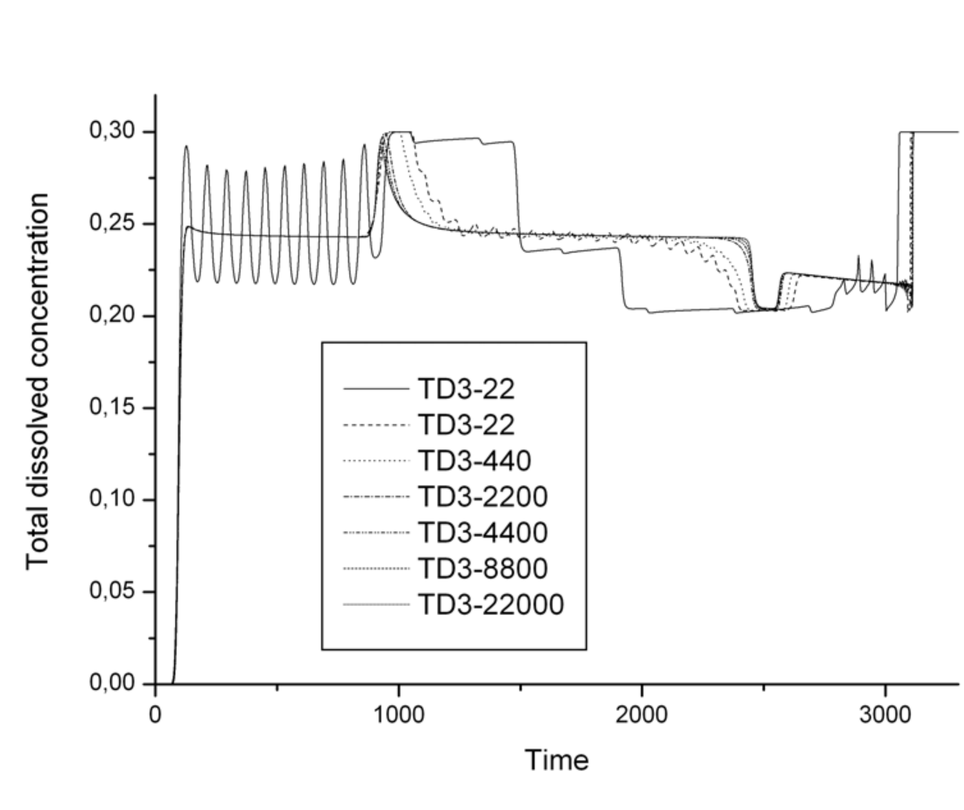
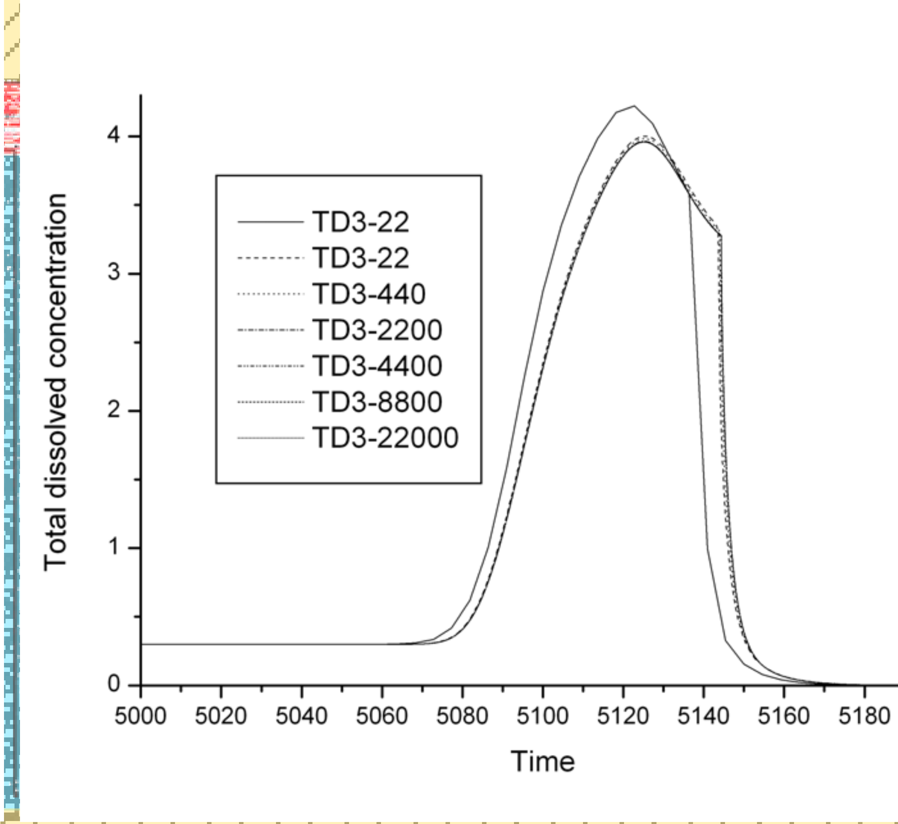
Elution curves for total X3





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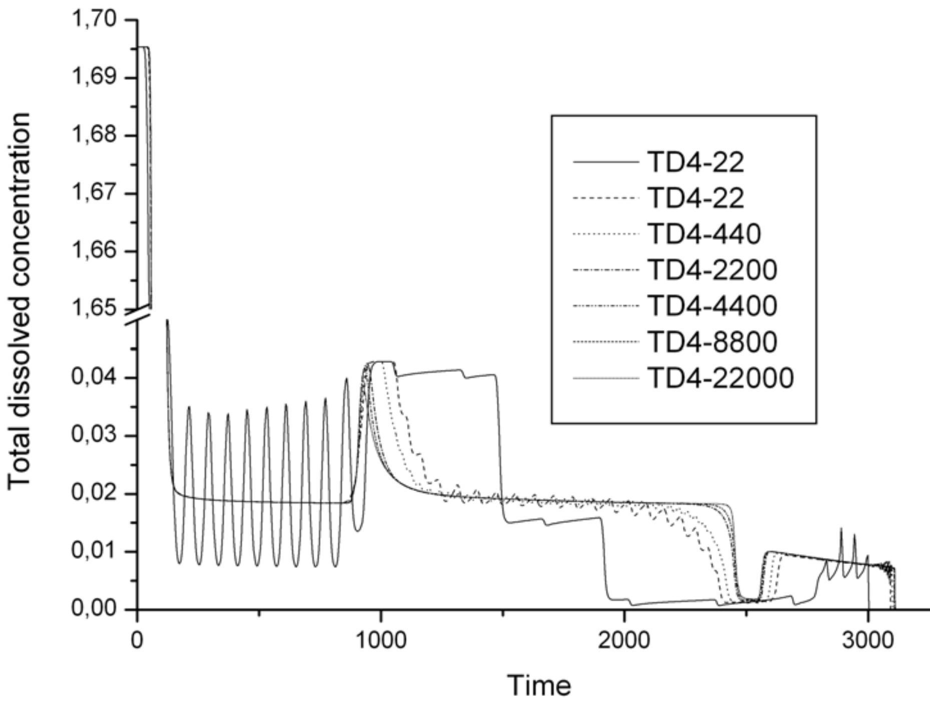
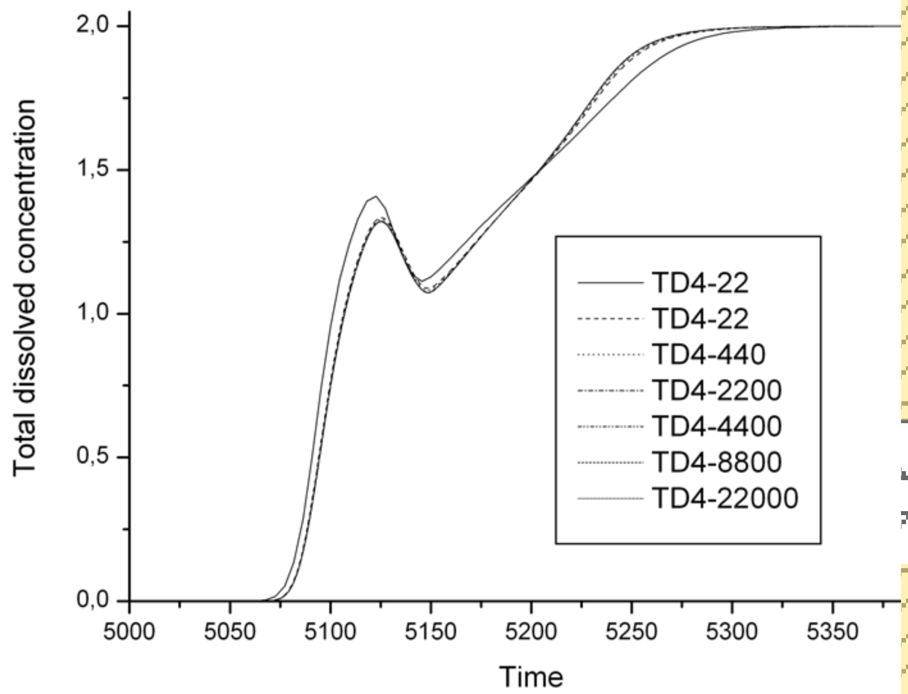
Elution curves for total X4





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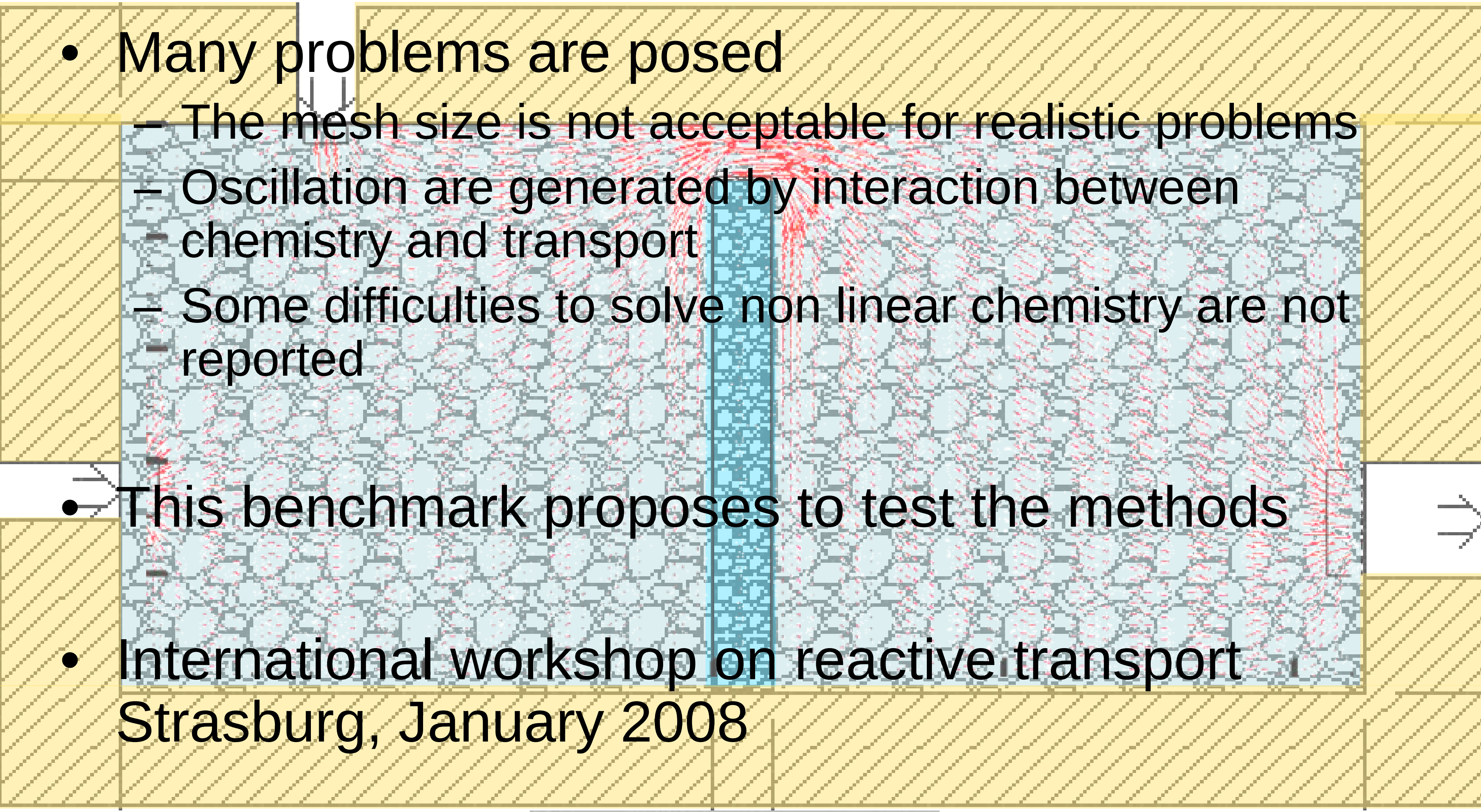
CONCLUSION ?



- Many problems are posed
  - The mesh size is not acceptable for realistic problems
  - Oscillation are generated by interaction between chemistry and transport
  - Some difficulties to solve non linear chemistry are not reported
- This benchmark proposes to test the methods
- International workshop on reactive transport Strasburg, January 2008

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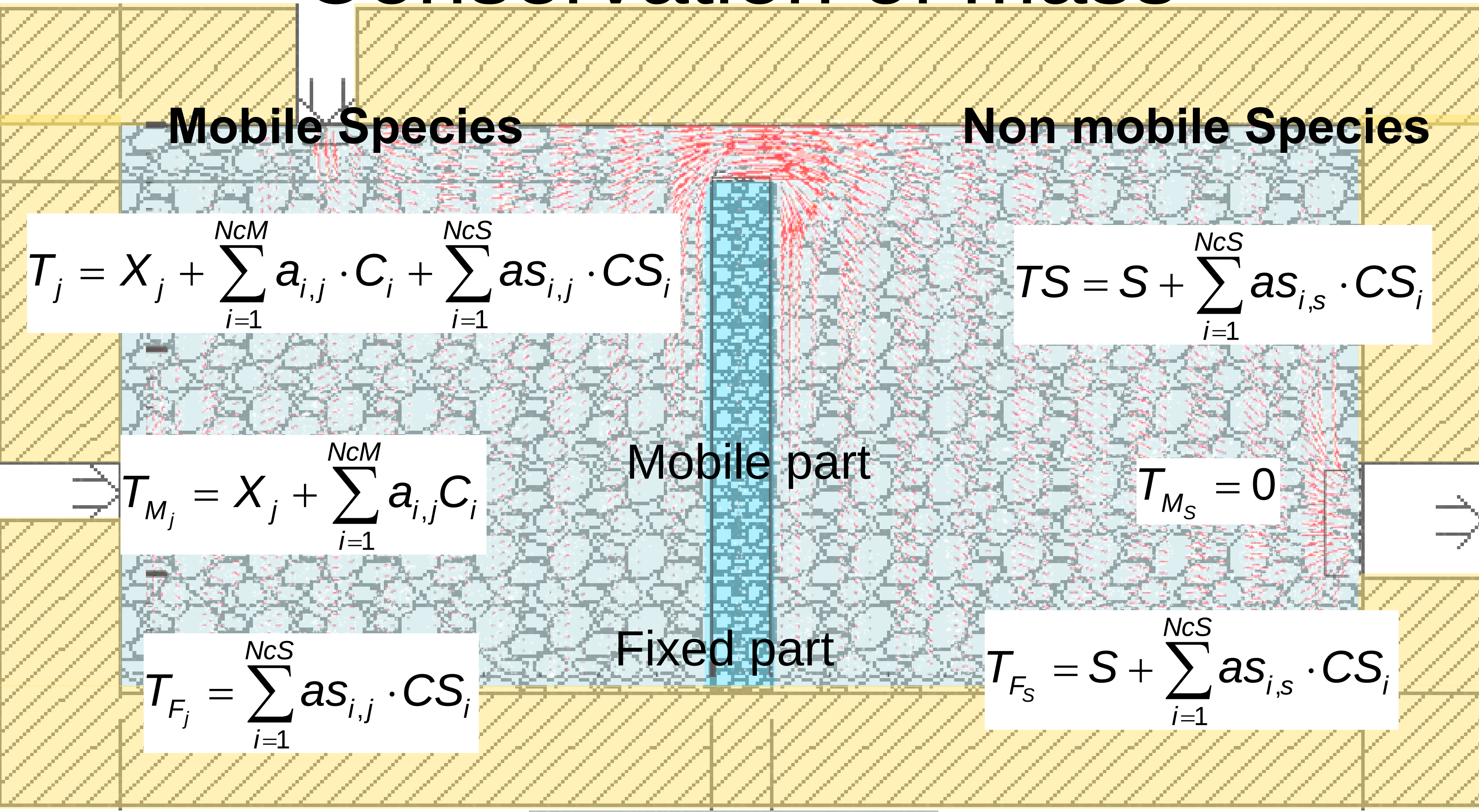
International workshop on reactive transport Strasbourg January 21-24 2008

- On day is devoted to the presentation of the benchmark results
- 10 000 € Reward for best participations to this benchmark

Conservation of mass



Mobile Species

$$T_j = X_j + \sum_{i=1}^{NcM} a_{i,j} \cdot C_i + \sum_{i=1}^{NcS} as_{i,j} \cdot CS_i$$

$$T_{M_j} = X_j + \sum_{i=1}^{NcM} a_{i,j} C_i$$

$$T_{F_j} = \sum_{i=1}^{NcS} as_{i,j} \cdot CS_i$$

Mobile part

Fixed part

Non mobile Species

$$TS = S + \sum_{i=1}^{NcS} as_{i,s} \cdot CS_i$$

$$T_{M_S} = 0$$

$$T_{F_S} = S + \sum_{i=1}^{NcS} as_{i,s} \cdot CS_i$$