The MoMaS Reactive Transport Benchmark
Presentation of the Models

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Modelling Reactive Transport in Porous Media

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Plan

Motivation

Design decisions

- Compare numerical methods and codes for reactive transport
- Bias towards nuclear waste disposal
- Fixed physical / chemical model
- Simple chemical system, with high numerical complexity
- No thermodynamic database

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Consequences

- Synthetic chemical system
- Small number of species / reactions
- Unrealistic stoichiometry, equilibrium constants
- Several levels of difficulty

Main questions

Space discretization

Features	Stability, numerical diffusion, efficiency
Methods	Finite element / volumes, Ellam, particles, ...

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- Explicit /implicit
- Lower /higher order
- Adaptive time step (heuristic, residual based)

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Coupling methods

Operator splitting To iterate or not to iterate, OS error control

Global DSA, DAE, Newton (non-linear system solution, linear algebra, ...)

CPU time, memory

Flow and Transport

Saturated flow : Darcy's law

$$\begin{cases} \omega u = -K \nabla h \\ \nabla.(\omega u) = 0 \end{cases}$$

ω porosity, u Darcy velocity

Transport model

$$\omega \frac{\partial \left(T_{M_j} + T_{F_j} \right)}{\partial t} + \nabla . \left(\omega u T_{M_j} \right) - \nabla . \left(D \nabla T_{M_j} \right) = -\omega \sum_k ac_{k,j} f_k(C_i, Cc_k)$$

Dispersion tensor $D = \alpha_T \, \omega \, |u| \, I + (\alpha_L - \alpha_T) \, \omega \frac{u \otimes u}{|u|}$

T_{M_j} (resp. T_{F_j}) total mobile (resp. immobile) for concentration component j, kinetic source term, rate $f_k(C_i, Cc_k)$

Chemical equilibrium

Reactions

$$\sum_{j=1}^{NxM} a_{ij} X_i \leftrightarrows C_i$$

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

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Mass action laws

$$C_i = K_i \prod_{j=1}^{NxM} X_j^{a_{ij}}$$

$$CS_i = Ks_i \prod_{j=1}^{NxM} X_j^{as_{ij}} S^{as_{is}}$$

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Conservation of mass

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

$$TS = S + \sum_{i=1}^{NcS} as_{is} CS_i$$

Kinetic reactions

Formation of immobile species Cc :

$$3C_3 \leftrightarrows \text{Cc} + 2X_4$$

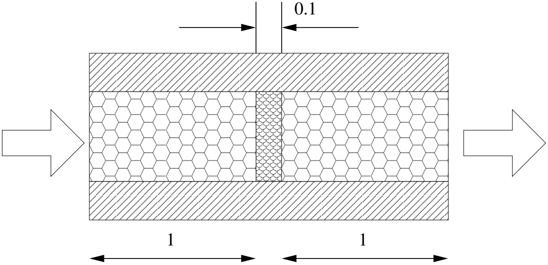
Rate law :

$$\frac{d\text{Cc}}{dt} = \left(0.2\frac{C_3^3}{X_4^2} - 1\right)k, \quad \text{with Cc} \geq 0,$$

$$k = \begin{cases} 10^{-2} & \text{if } 0.2\dfrac{C_3^3}{X_4^2} \geq 1 \\ 10 & \text{otherwise.} \end{cases}$$

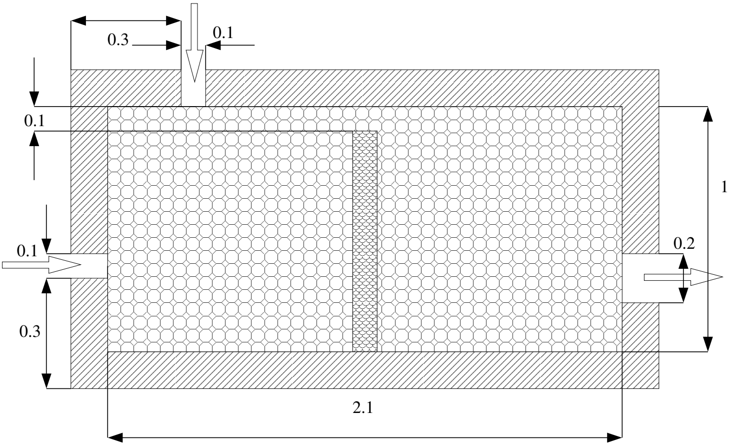
Initial condition : $\text{Cc}(t = 0) = 5$.

Geometry : 1D model



	Medium A	Medium B
Porosity $\omega[-]$	0.25	0.5
Permeability K (LT^{-1})	10^{-2}	10^{-5}
Dispersivity α_L[L]	10^{-2} (10)	$6\,10^{-2}$ (60)
Dispersivity α_T[L]	10^{-3} (1)	$6\,10^{-3}$ (6)
Concentration T_s	1	10

Geometry : 2D model



Chemistry : easy test case

Morel tableau

	X_1	X_2	X_3	X_4	S	K
C_1	0	-1	0	0	0	10^{-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	10^{35}
CS_1	0	3	1	0	1	10^{6}
CS_2	0	-3	0	1	2	10^{-1}
Total	T_1	T_2	T_3	T_4	TS	
Init. medium A (B)	0	-2	0	2	1 (10)	
injection $t \in [0, 5000]$	0.3	0.3	0.3	0		
Leaching $t \geq 5000$	0	-2	0	2		

Chemistry : medium test case

Morel tableau

	X_1	X_2	X_3	X_4	S	K
C_1	0	-1	0	0	0	10^{-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	10^{35}
C_6	0	10	3	0	0	10^{32}
C_7	0	-8	0	2	0	10^{-4}
CS_1	0	3	1	0	1	10^{6}
CS_2	0	-3	0	1	2	10^{-1}
Total	T_1	T_2	T_3	T_4	TS	
Init. medium A (B)	0	$-3\,(-9)$	0	1 (3)	1 (10)	
injection $t \in [0, 5000]$	0.3	0.3	0.3	0		
Leaching $t \geq 5000$	0	-3	0	1.5		

Morel tableau

	X_1	X_2	X_3	X_4	X_5	S	K
C_1	0	-1	0	0	0	0	10^{-12}
C_2	0	1	1	0	0	0	1
C_3	0	-1	0	1	0	0	1
C_4	0	-4	1	3	0	0	0.1
C_5	0	4	3	1	0	0	10^{35}
C_6	0	10	3	0	0	0	10^{32}
C_7	0	-8	0	2	0	0	10^{-4}
CS_2	0	-3	0	1	0	2	10^{-1}
CP_1	0	3	1	0	0	0	10^{10}
CP_2	0	1	0	0	1	0	20
Total	T_1	T_2	T_3	T_4	T_5	TS	
Init. A (B)	0	$-30\,(-90)$	0	10 (30)	0	1 (10)	
inj.	0.3	0.3	0	0		0.3	
Leach.	0	-3	0	1.5	0		

Conclusions

Main difficulties

- Very large difference in the size of equilibrium constants
- Large stoichiometric coefficients, gives very nonlinear behavior
- Long simulation time
- Correct resolution of transport for 2D case

Limitations

- Artificial chemistry, unrealistic ?
- Easy subset aimed at mathematicians
- Only one situation, limited conclusions