A Finite Volume Scheme for the Transport of Radionucleides in Porous Media

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Physical problems

Transport of mass and energy within porous media :

- Pollution of soils
- Degradation of concrete
- Migration of hydrocarbon components
- ...

Examples of conservation equations in porous media

N^c components, N_p phases

$$(A_p^c)_t + \mathrm{div} F_p^c = R_p^c$$

$$A_p^c = S_p \xi_p X_p^c$$

$$F_p^c = \xi_p X_p^c V_p - D_p^c(V_p) \cdot \nabla X_p^c$$

$$D_p^c(v) \cdot w = a_p^c w + |v| \left(b_p^c \tfrac{v \cdot w}{v \cdot v} v + c_p^c (w - \tfrac{v \cdot w}{v \cdot v} v) \right)$$

$$V_p = -K \tfrac{k_{rp}(S_p)}{\mu_p} (\nabla P_p - \rho_p g)$$

Mathematical questions

Existence and uniqueness of solutions

Numerical approximation

Convergence and error estimates

...

Approximation using finite volume methods

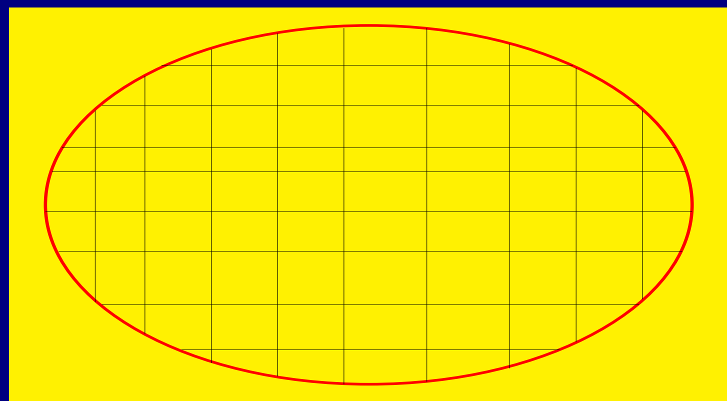
Conservation equation

$$\boxed{\frac{\partial A}{\partial t} + \mathrm{div}\mathbf{F} = R}$$

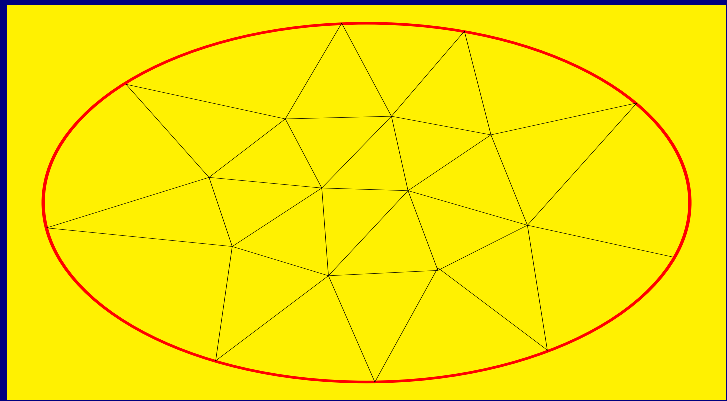
with

- A : extensive quantity
- F : flux
- R : reaction term

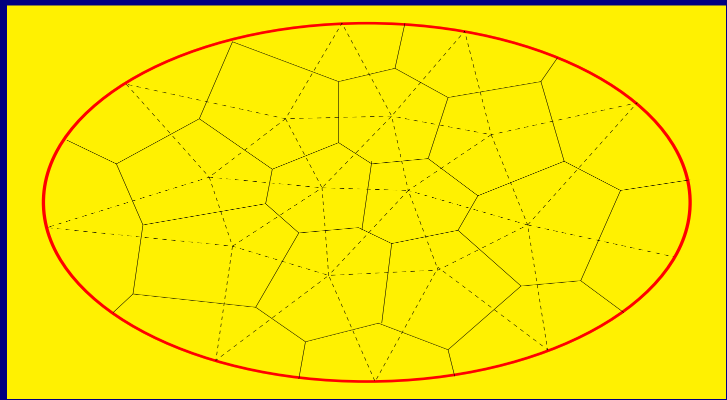
Partition of the domain



Partition of the domain



Dual mesh (Voronoï mesh)



Extensive balance in control volumes

$$m_K \frac{A_K^{(n+1)} - A_K^{(n)}}{\delta t^{(n)}} + \sum_{L \in \mathcal{N}_K} F_{K,L}^{(n,n+1)} = m_K R_K^{(n)}$$

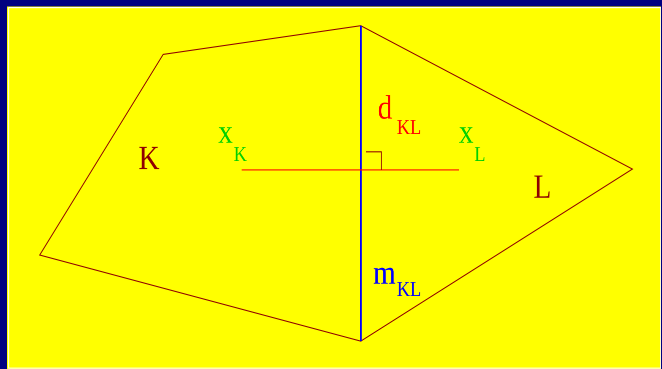
$F_{K,L}^{(n,n+1)}$ approx. $\frac{1}{\delta t^{(n)}} \int_{t^{(n)}}^{t^{(n+1)}} \int_{K|L} \mathbf{F} \cdot \mathbf{n}_{K,L} \, ds dt$

$F_{K,L}^{(n,n+1)} = -F_{L,K}^{(n,n+1)}$ $\Rightarrow$ local conservation

Flux approximation

Finite Difference Approximation of $\mathbf{F} = -a \, \nabla u$

$$F_{K,L} = -a \; m_{KL} \frac{u_L - u_K}{d_{KL}}$$



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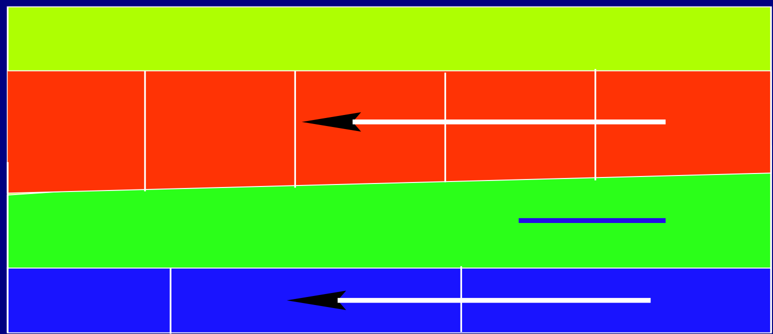
The COUPLEX 1 case

$$\mathrm{div} V_1 = 0 \textbf{ with } V_1 = -K(\nabla P_1 - \rho_1 g)$$
$$(X_1^1)_t - \mathrm{div}\left(\; X_1^1 V_1 - D(V_1)\cdot \nabla X_1^1 \; \right) = -\Lambda X_1^1$$



Finite volume scheme on Voronoï mesh

$H_K = P_{1K} - \rho_1 g \cdot z_K$ **and** $V_{K,L} = m_{KL} \frac{H_K - H_L}{d_{KL}}$

FV scheme: $\sum_{L \in N_K} V_{K,L} = 0$

$$\frac{m_{KL}}{d_{KL}} = -\int_\Omega \nabla \varphi_K(x) \cdot \nabla \varphi_L(x) dx$$ $\Rightarrow$ **FV = FE**

approx. ∇H constant by triangle

Finite volume scheme for concentrations

$$m_K \frac{X_K^{(n+1)} - X_K^{(n)}}{\delta t} + \sum_{L \in N_K} \left[\begin{array}{c} X_{K,L}^{(m)} V_{K,L} - \\ D_{KL}(X_L^{(m)} - X_K^{(m)}) \end{array} \right] =$$
$$m_K (R_K^{(n)} - k X_K^{(n+1)})$$

with

$$D_{KL} = -\int_\Omega \nabla \varphi_K(x) D(\nabla H) \nabla \varphi_L(x) dx$$

$m = n$ or $m = n + 1$

Upwinding scheme

if $V_{K,L} \geq 0$	then	$X_{K,L}^{(m)} = X_K^{(m)}$
	else	$X_{K,L}^{(m)} = X_L^{(m)}$

Variable Péclet number finite volume scheme

$$X_{K,L}^{(m)} = \theta_{K,L} X_K^{(m)} + (1 - \theta_{K,L}) X_L^{(m)}$$
$$\Rightarrow F_{K,L}^{(m)} = \left(\theta_{K,L} X_K^{(m)} + (1 - \theta_{K,L}) X_L^{(m)}\right) V_{K,L} -$$
$$D_{KL}(X_L^{(m)} - X_K^{(m)})$$

minimum of $|\theta_{K,L} - \frac{1}{2}|$ **with** $\theta_{K,L} \in [0, 1]$ **and**

$\theta_{K,L} V_{K,L} + D_{KL} \geq 0$, $(1 - \theta_{K,L}) V_{K,L} - D_{KL} \leq 0$

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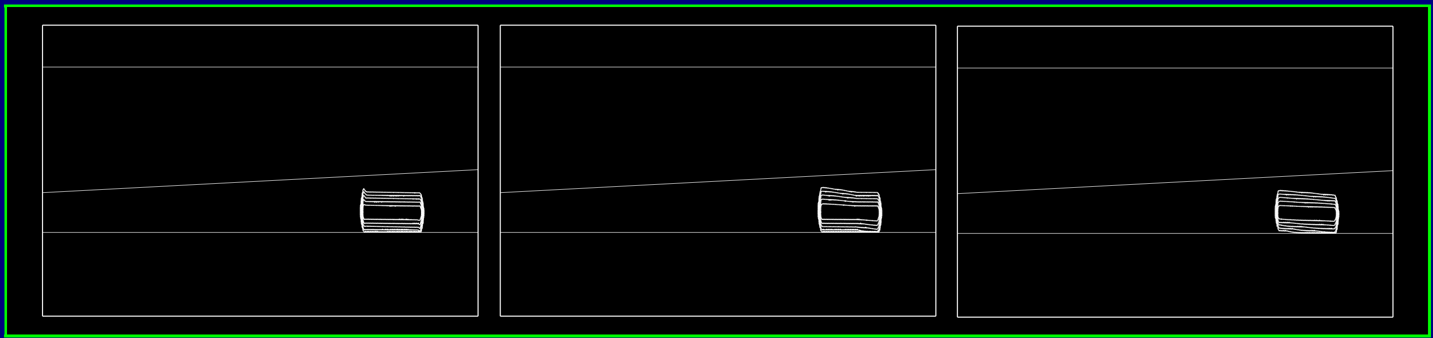
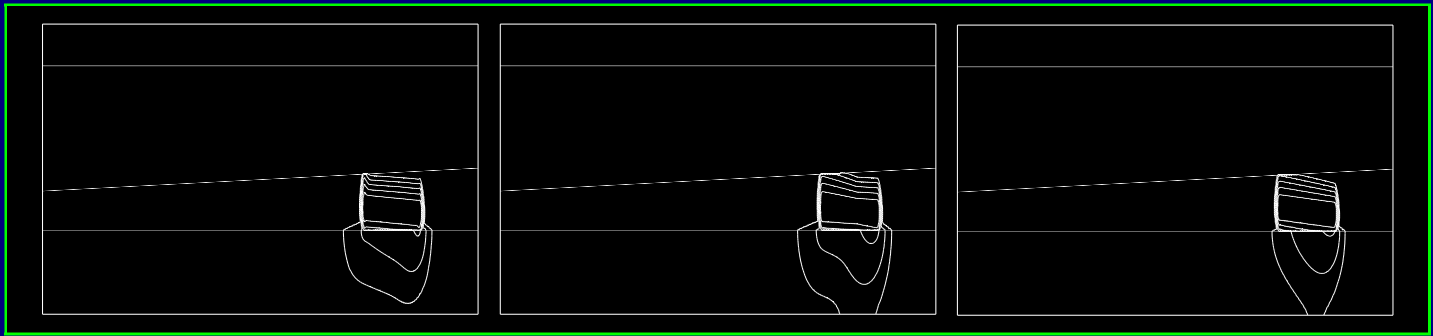
Contour levels of iodine at $10110\ years$



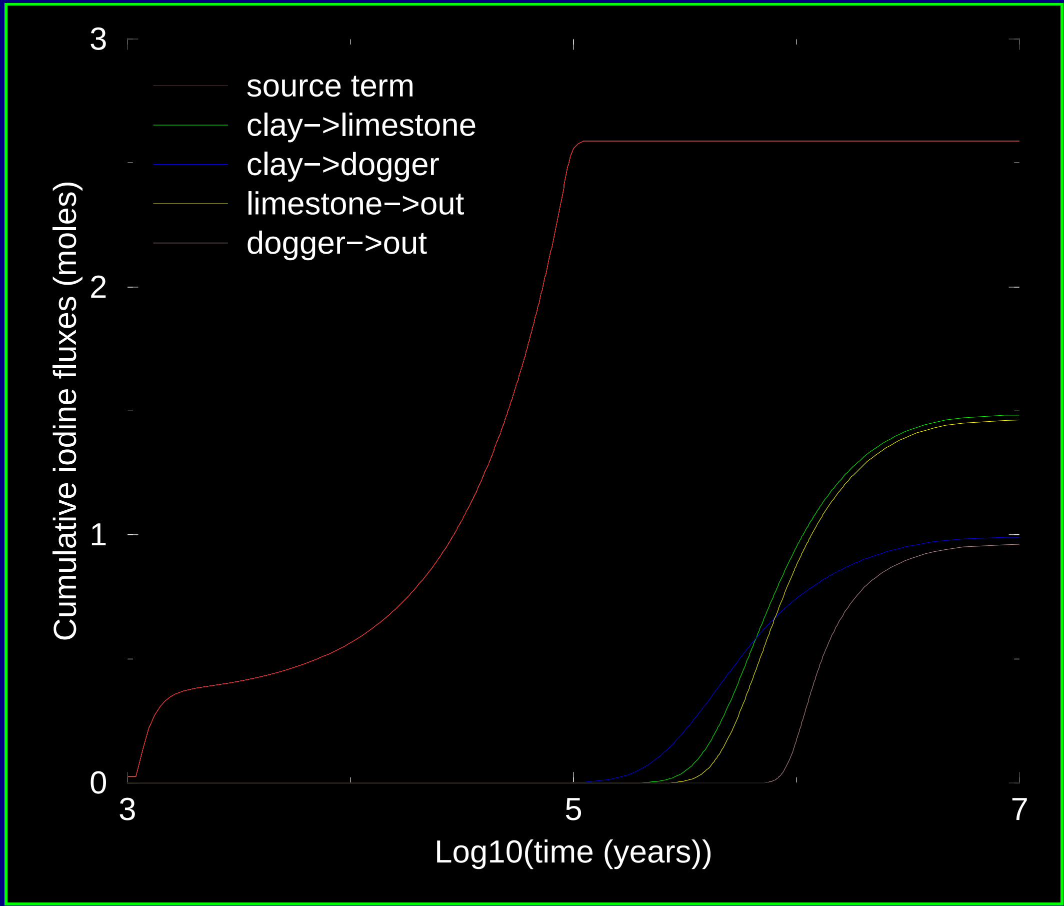
MUSCL exp. (left), up.imp. (middle), Péc.imp. (right)

Contour levels of iodine at $50110\ years$



MUSCL exp. (left), up.imp. (middle), Péc.imp. (right)

Cumulative total fluxes of iodine



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Concluding remarks

1. FV simple and accurate = industrial schemes.
2. A complete engineering approach ? Handling uncertainties on
   - (a) porosity, permeability, diffusivity fields, source terms,
   - (b) boundary conditions as function of time.