

Enfouissement du CO₂: aspects physiques, numériques et mathématiques

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Simulation du stockage géologique du CO₂

■ Objectifs

- Optimisation de l'injection du CO₂
- Optimisation du stockage du CO₂
- Prédiction et réduction des risques

■ Modèles

- Ecoulements polyphasiques compositionnels
- Interactions eau – roche
- Géomécanique

Stockage du CO₂ dans les aquifères salins

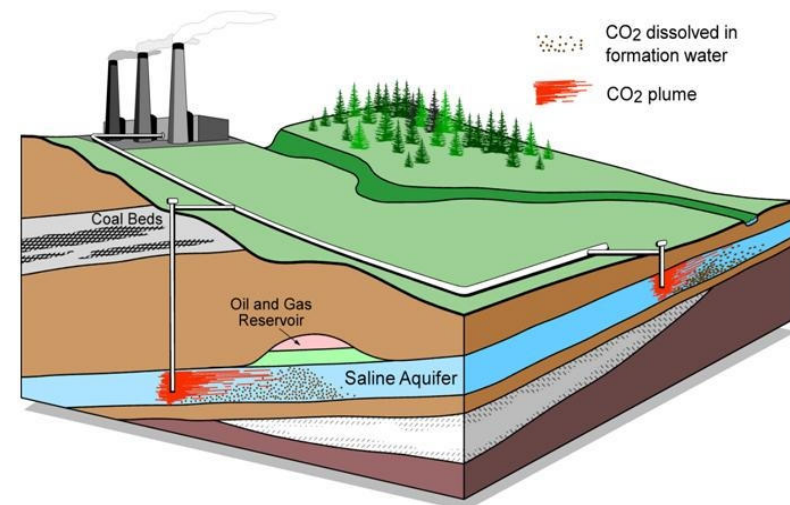
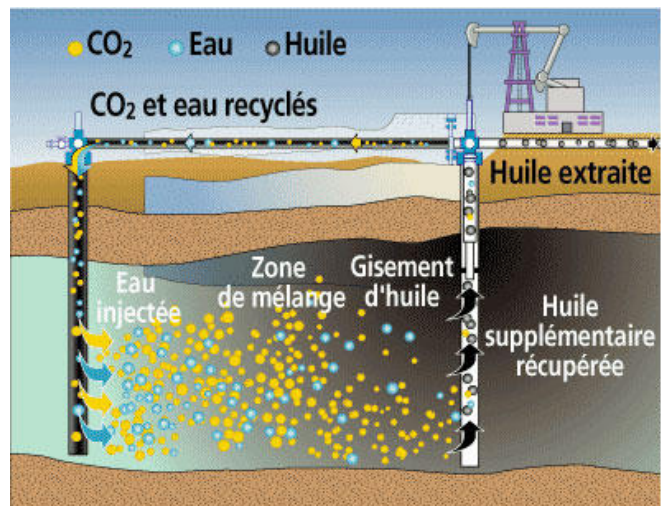
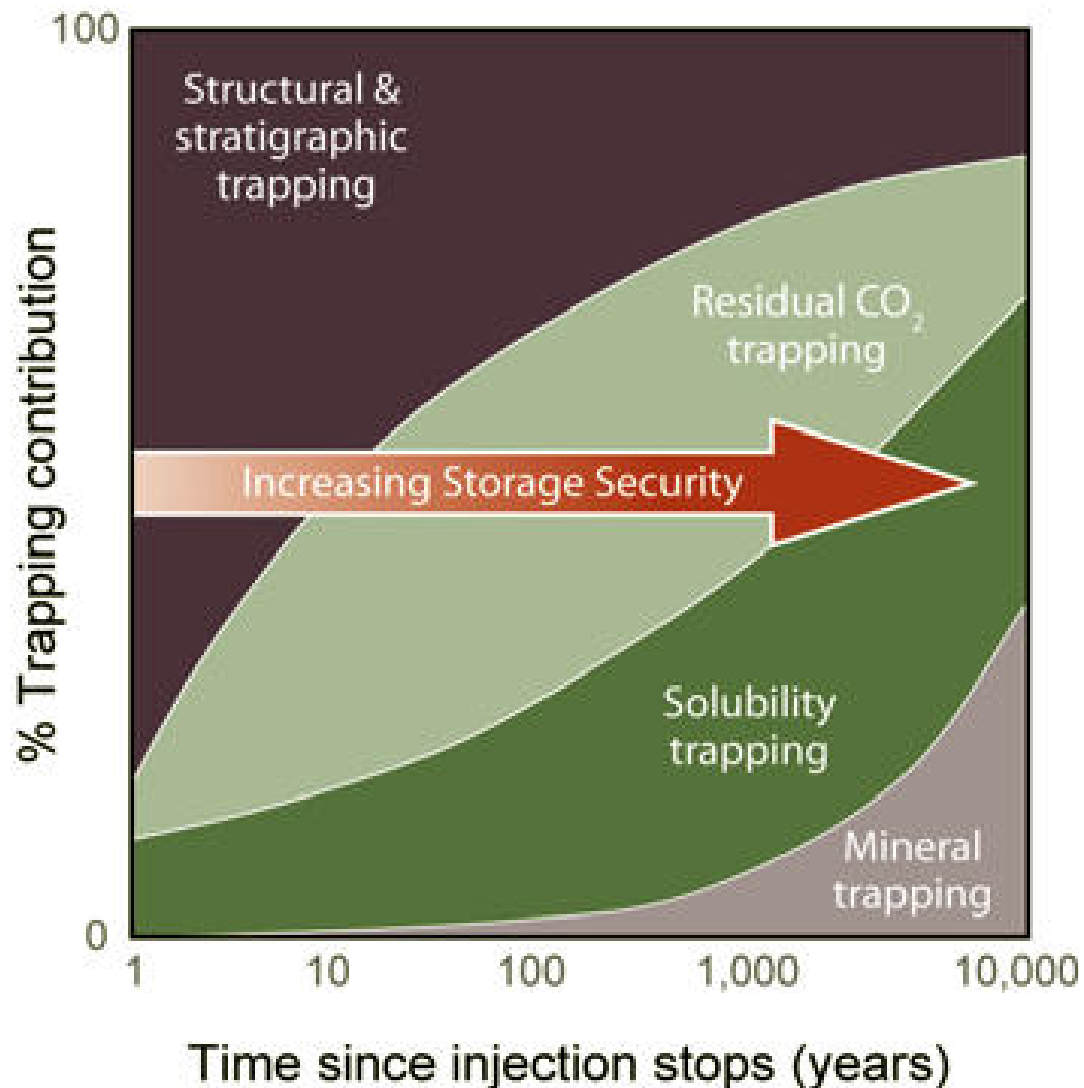


Figure 1.



Production d'huile par injection de CO₂

Modes de stockage en fonction du temps

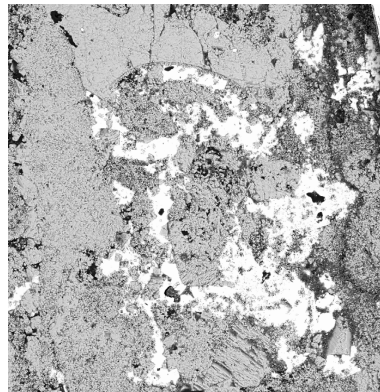
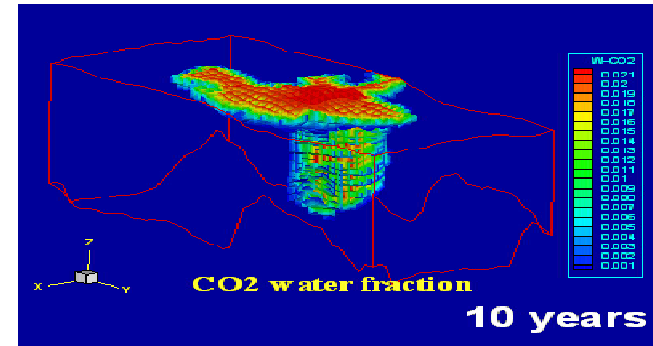
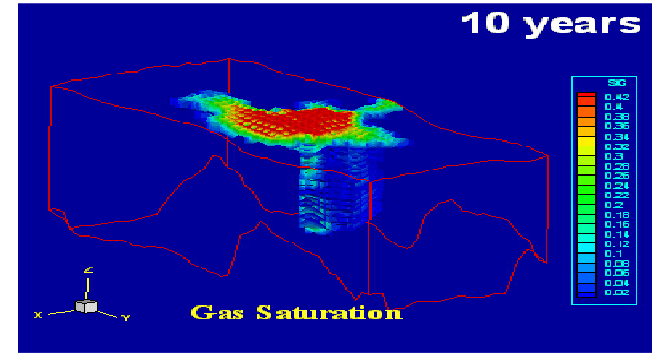
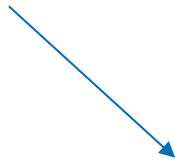


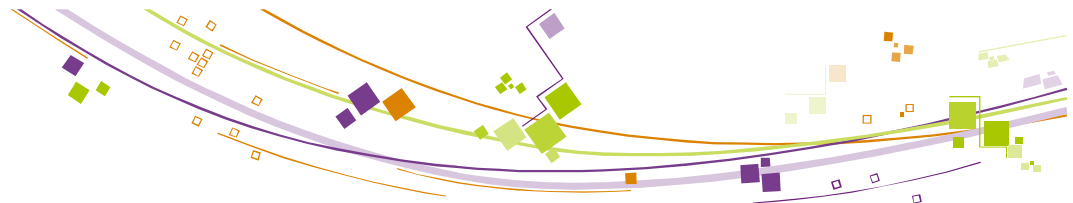
- Stockage géologique
- Stockage capillaire
- Dissolution dans la phase eau
 - CO₂(aq), HCO₃⁻, CaHCO₃⁺, MgHCO₃⁺, NaHCO₃⁰, ...
- Stockage minéral
 - CaCO₃ (calcite), FeCO₃ (siderite), NaAlCO₃(OH)₂...

Phase d'injection du CO2: 10 à 50 ans



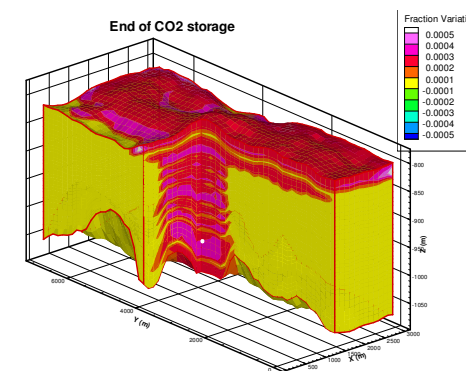
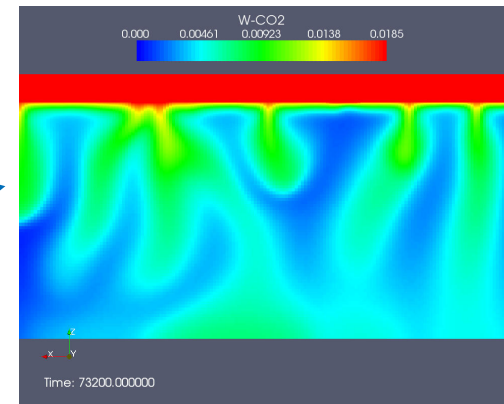
- Darcy diphasique: gradient de pression et gravité
- Dissolution du CO2 dans l'eau
- Altération proche puits
- Thermique
- Géomécanique
 - Couverture
 - Failles



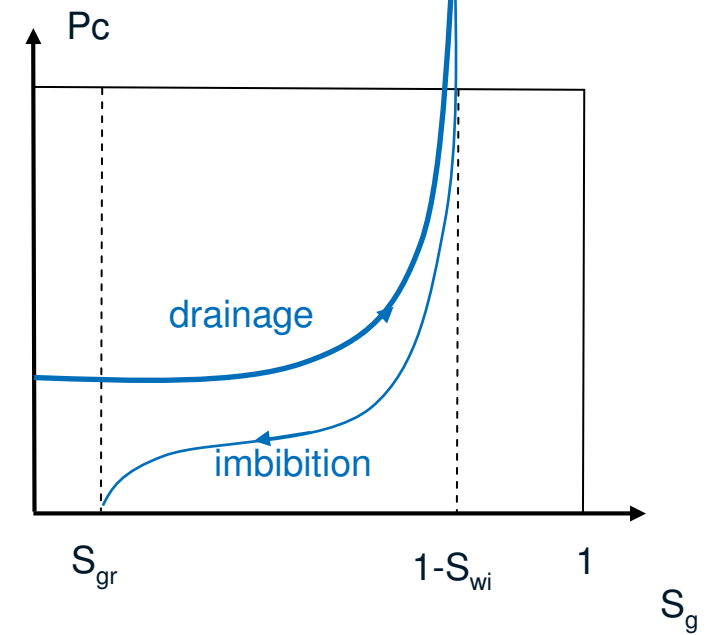
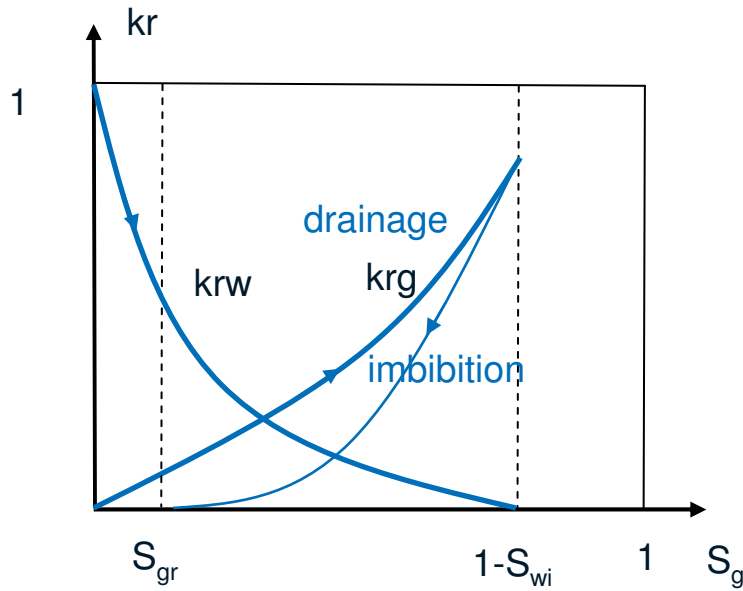
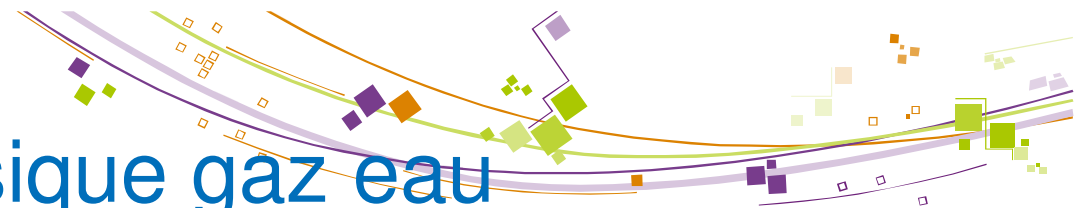


Phase de stockage: 10 à 50 ans – 10000 ans

- Piégeage capillaire
- Dissolution due aux instabilités gravitaires
- Convection diffusion-dispersion des espèces aqueuses
- Interactions eau – roches
- Fuites: failles, puits, couverture



Ecoulement diphasique gaz eau



$$\vec{V}_w = -\frac{kr_w(S_w)}{\mu_w} K(\nabla P_w - \rho_w \vec{g})$$

$$\vec{V}_g = -\frac{kr_g(S_g)}{\mu_g} K(\nabla P_g - \rho_g \vec{g})$$

$$P_g - P_w = P_c(S_g)$$

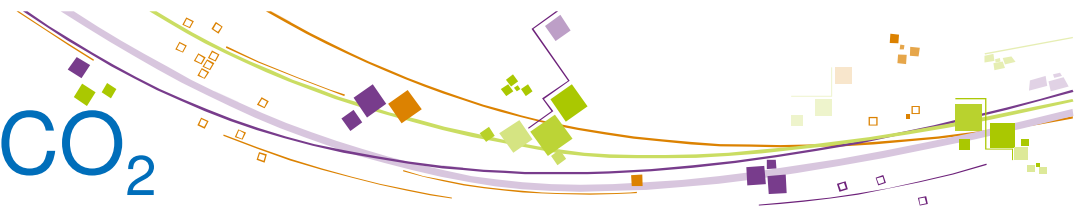
Écoulement diphasique avec dissolution du CO₂ dans l'eau

$$\left\{ \begin{array}{l} \partial_t \phi \left(\rho^w S^w C_{H_2O}^w \right) + \operatorname{div} \left(C_{H_2O}^w \rho^w \mathbf{V}^w \right) \\ \quad + \operatorname{div} \left(-\phi \rho^w S^w D^w \nabla C_{H_2O}^w \right) = 0, \\ \\ \partial_t \phi \left(\rho^w S^w C_{CO_2}^w + \rho^g S^g \right) + \operatorname{div} \left(C_{CO_2}^w \rho^w \mathbf{V}^w + \rho^g \mathbf{V}^g \right) \\ \quad + \operatorname{div} \left(-\phi \rho^w S^w D^w \nabla C_{CO_2}^w \right) = 0 \end{array} \right.$$

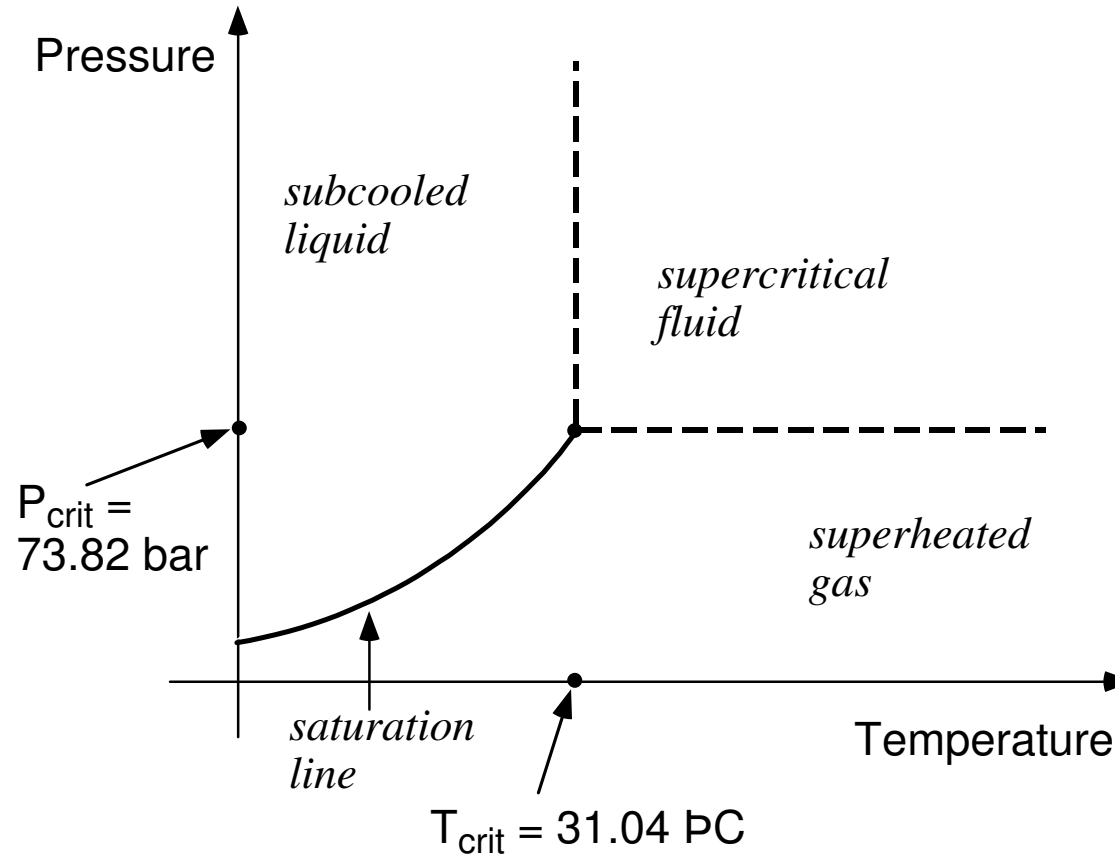
$$\left\{ \begin{array}{l} S^w + S^g = 1, \\ C_{H_2O}^w + C_{CO_2}^w = 1, \\ \left(C_{CO_2}^w - K_{CO_2} \right) S^g = 0, \\ C_{CO_2}^w \leq K_{CO_2}, \quad S^g \geq 0 \end{array} \right.$$

$$\rho^w(P, T, C^w), \quad \mu^w(P, T, C^w), \quad \rho^g(P, T), \quad \mu^g(P, T), \quad K_{CO_2}(P, T)$$

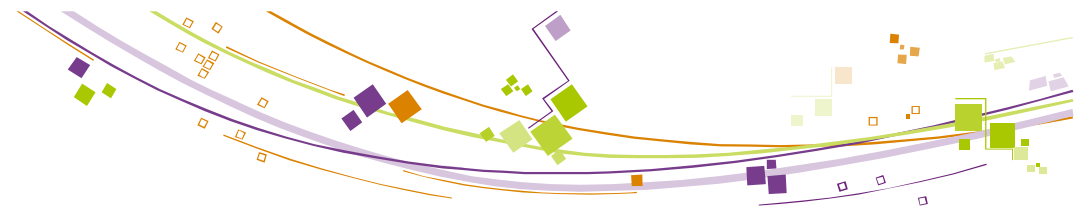
Phase diagram for CO₂



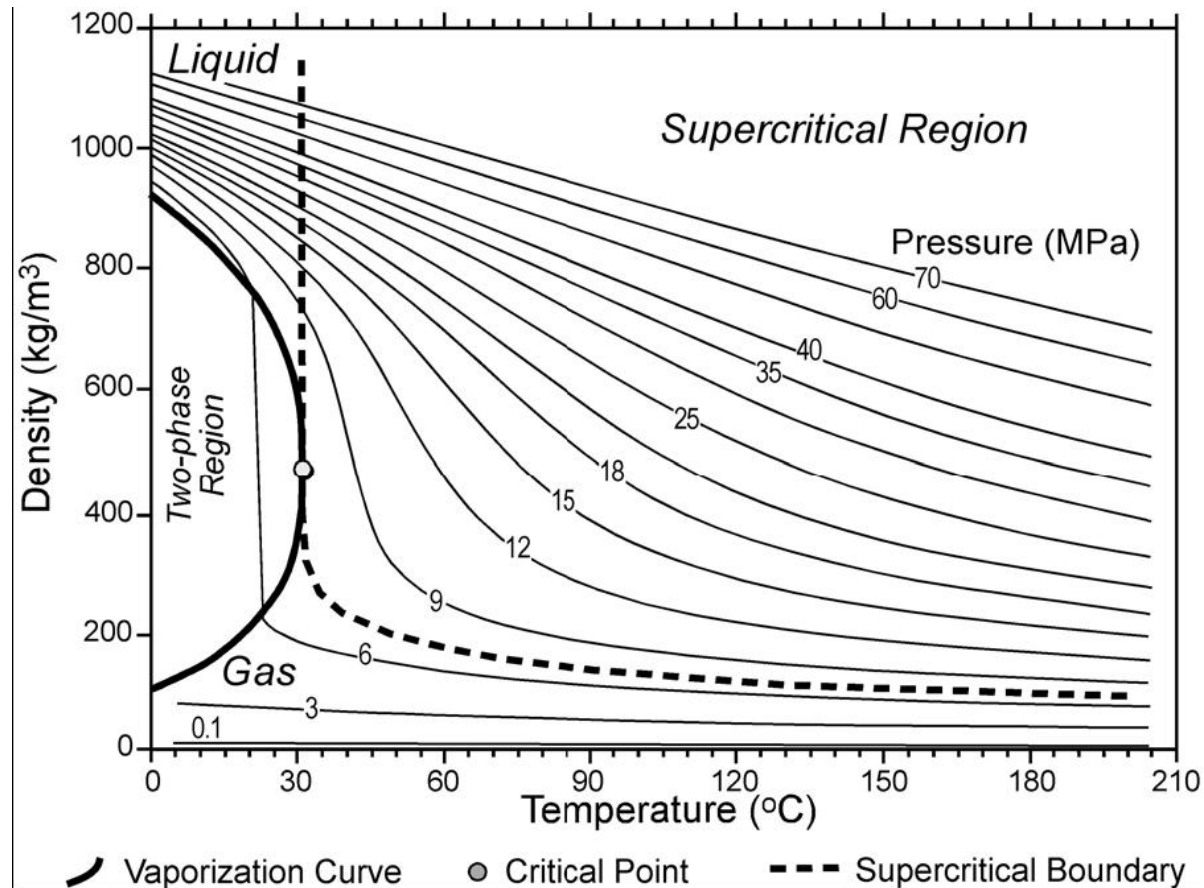
- CO₂ phase change is very sensitive to P and T encountered in natural conditions



(K. Pruess, LBNL)



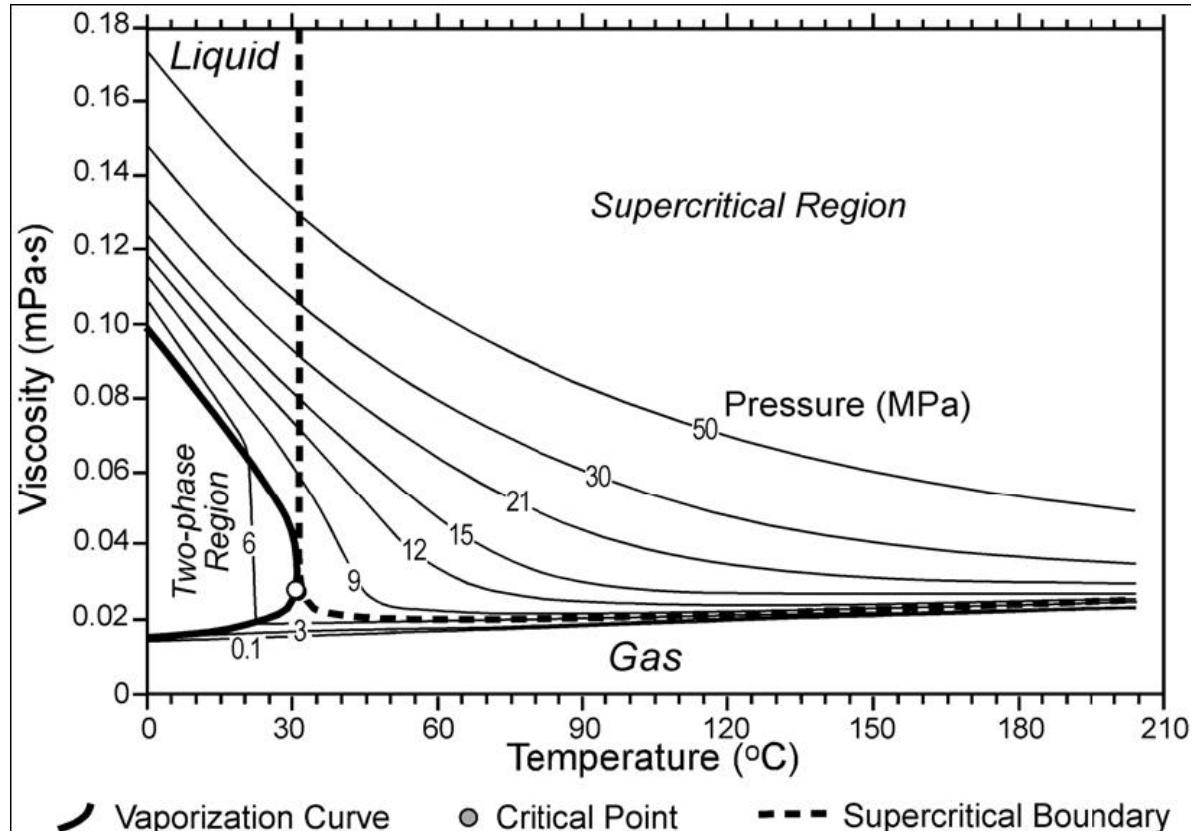
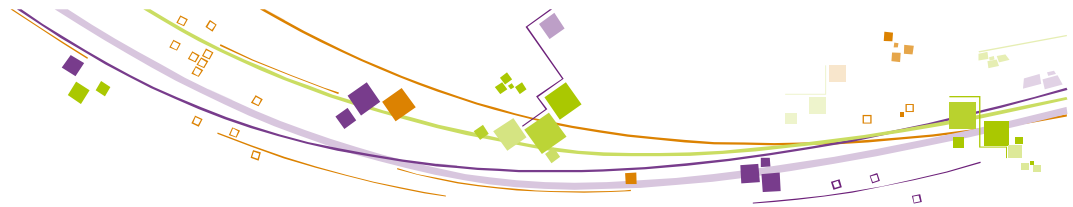
Density relation P & T



Density is increasing with pressure and decreasing with temperature.

The CO₂ as a supercritical state is lighter than brines (salted water) and therefore tends to move upward.

Viscosity

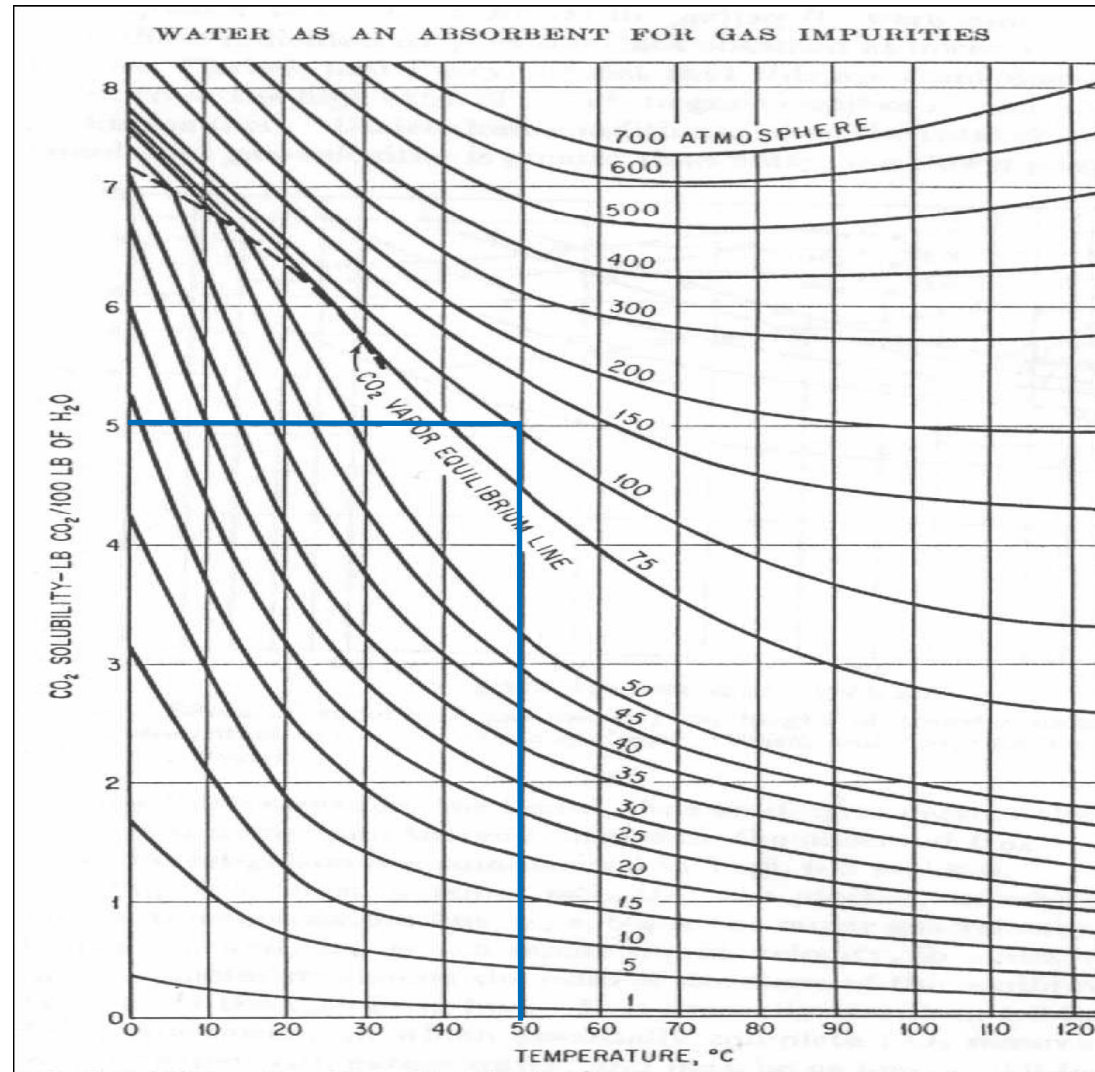


At higher temperatures there is a lower viscosity. A lower viscosity means a lower resistance to flow and thus CO2 can be injected better in this case.

Solubility

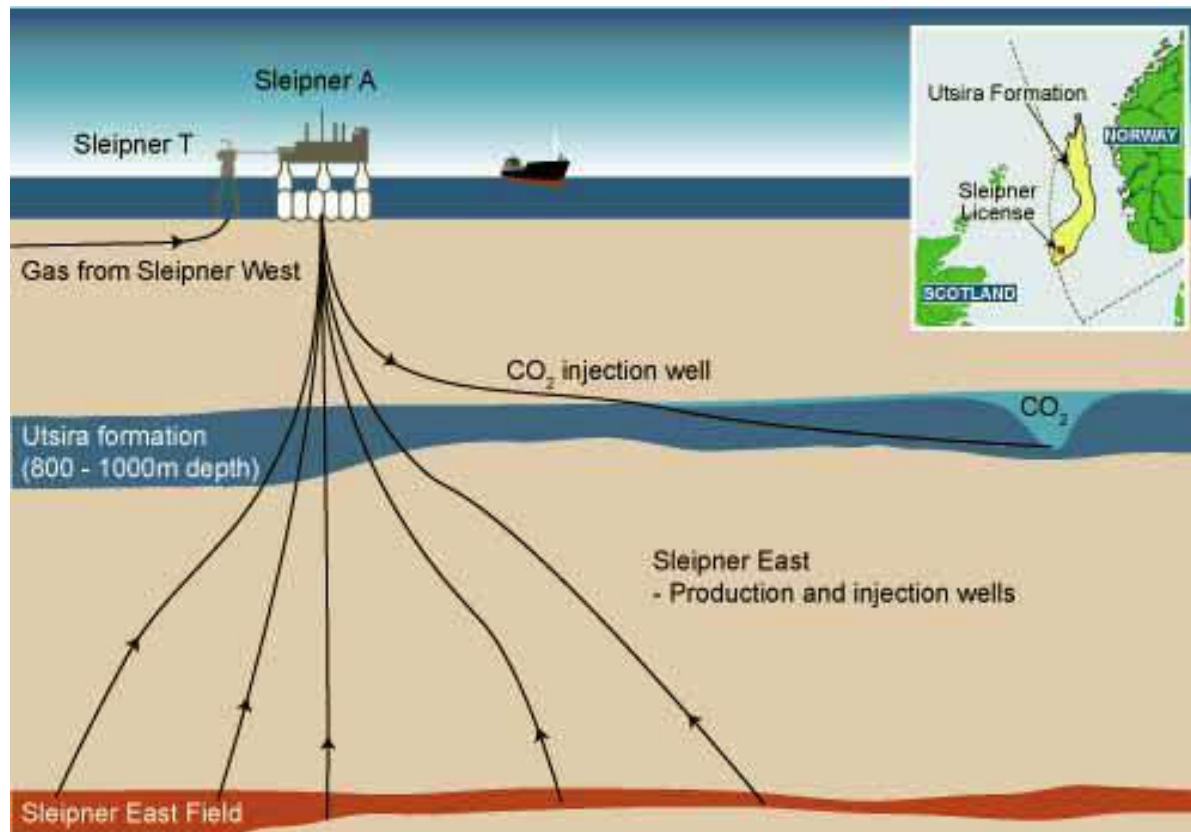
Solubility is also increasing with pressure and decreasing with temperature

In brines, CO₂ solubility decreases when salinity increases (salting-out effect)



at 100 bar and 50 °C, 50 Kg CO₂ can be dissolved in 1 cubic meter water

The Sleipner CO₂ storage project



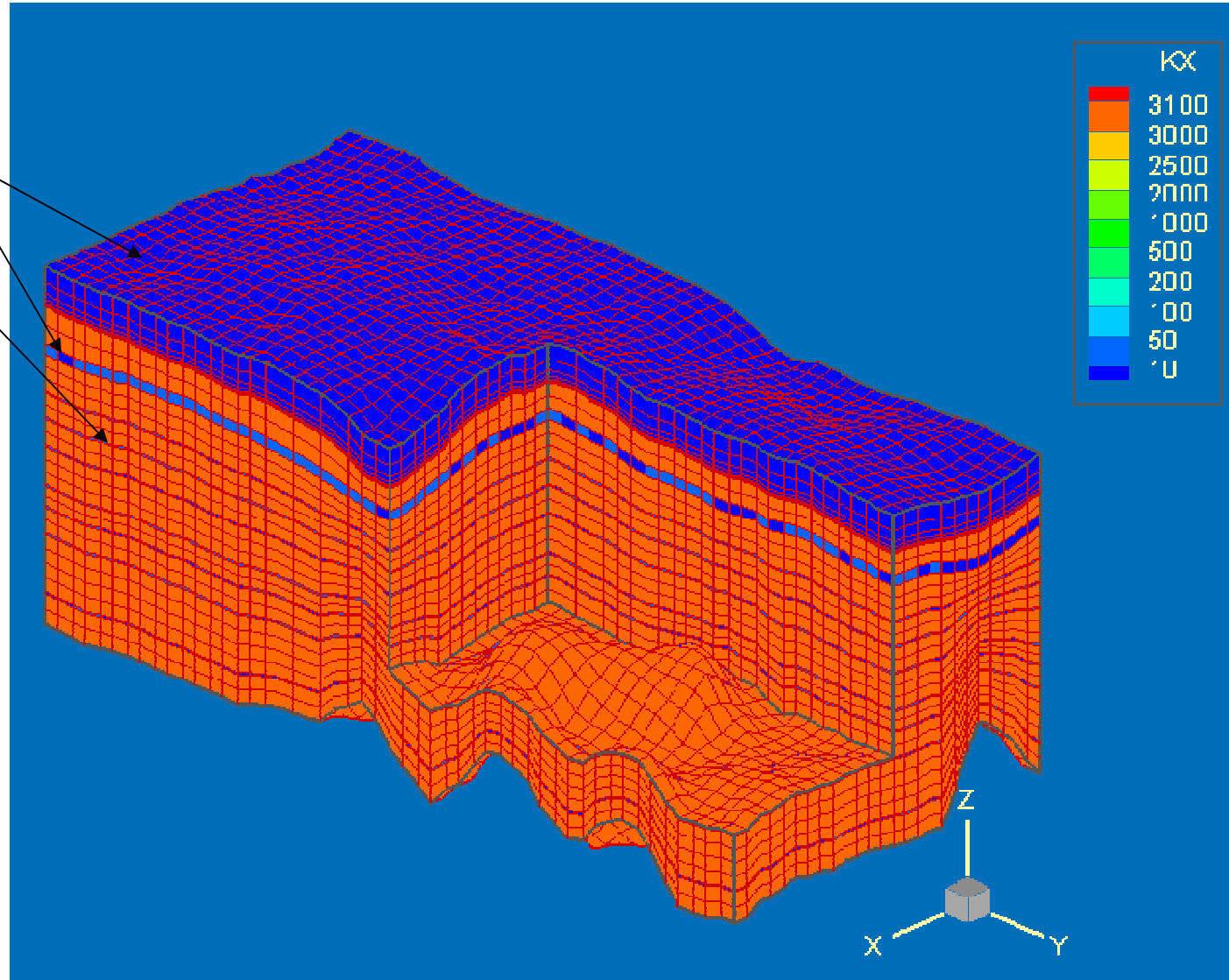
Opérateur : Statoil

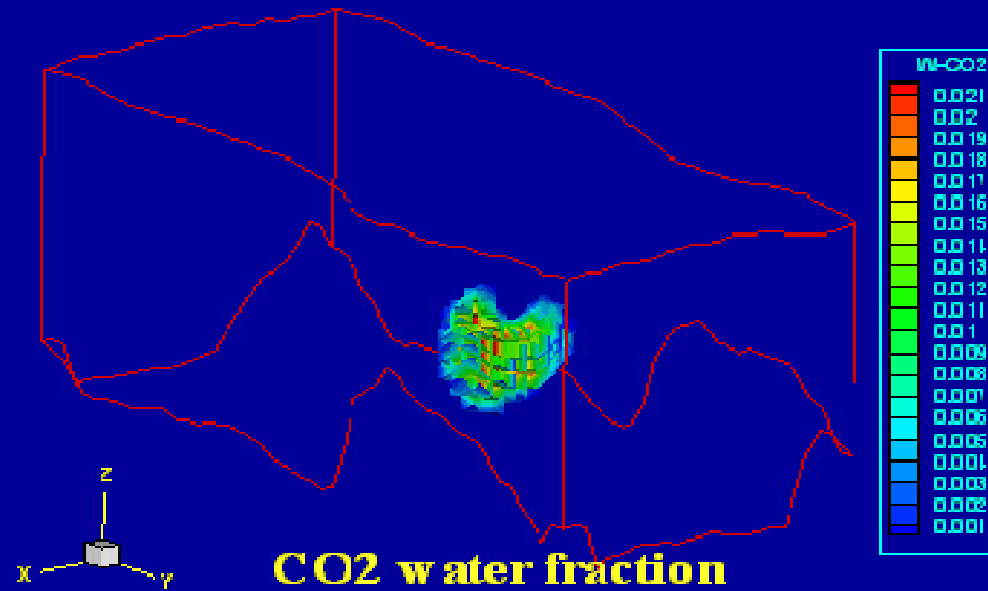
1 Mt CO₂ / an



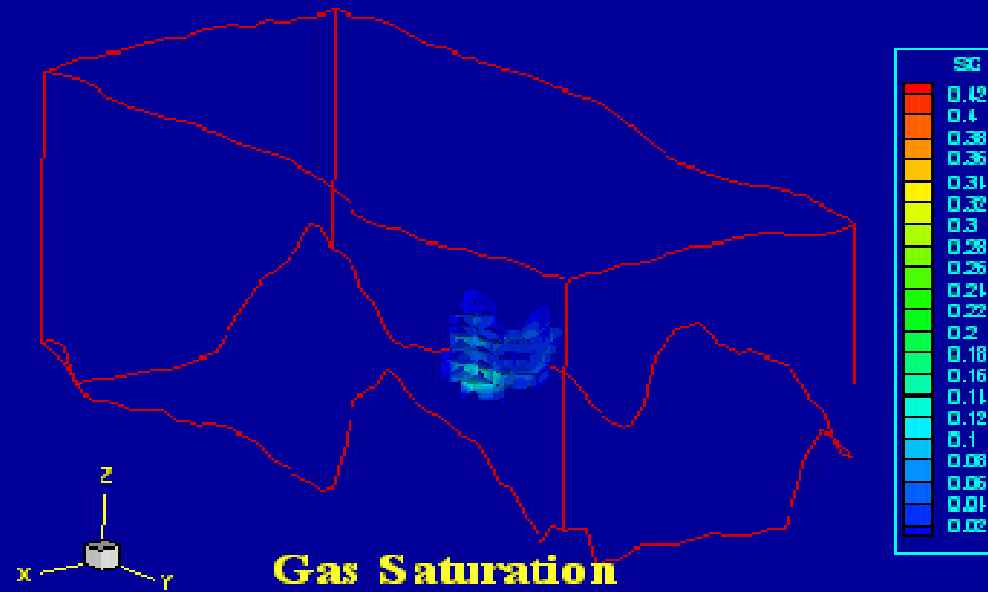
- 90 bars au sommet
- 37 °C
- Barrière imperméable au sommet
- CL hydrostatique latérale

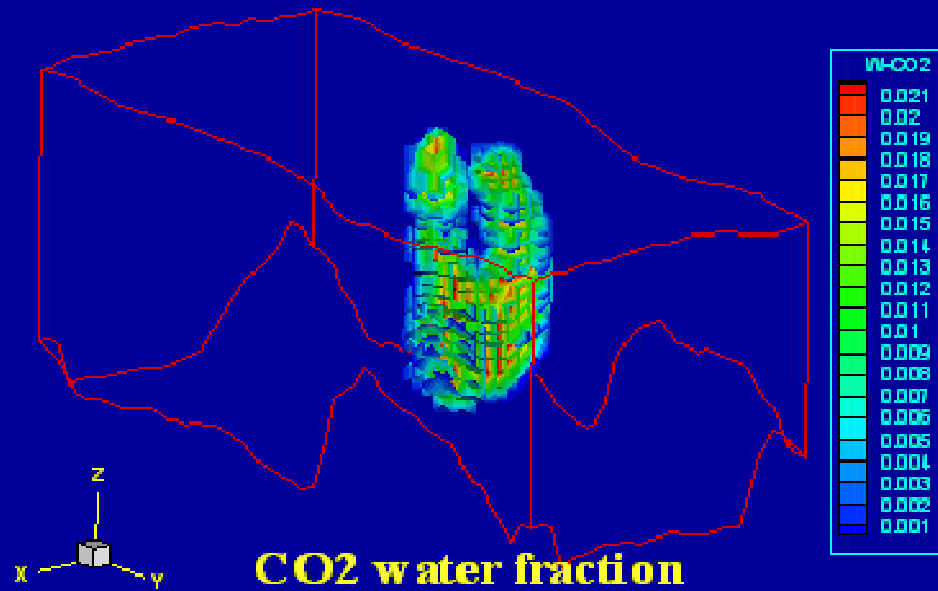
Argile
Sable



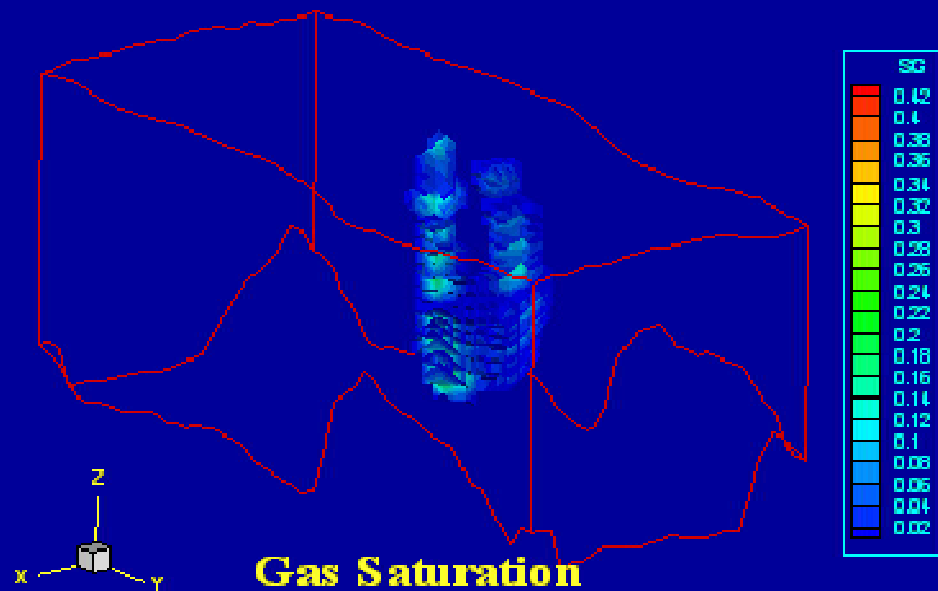


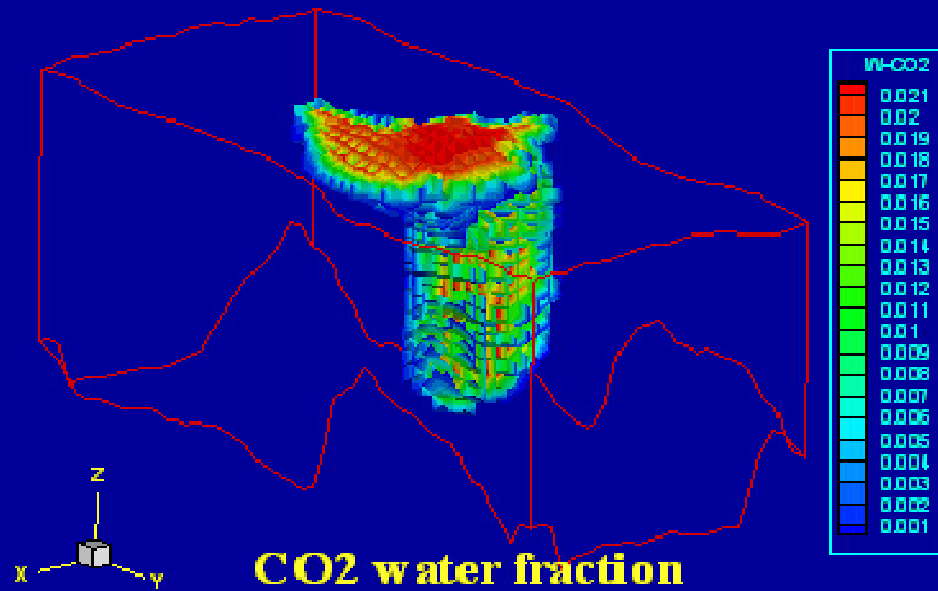
1 year



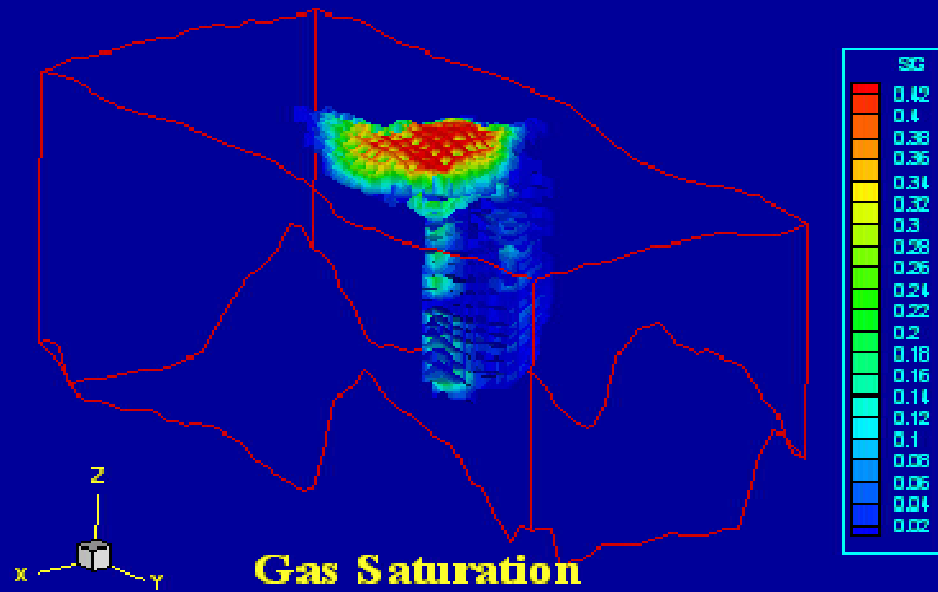


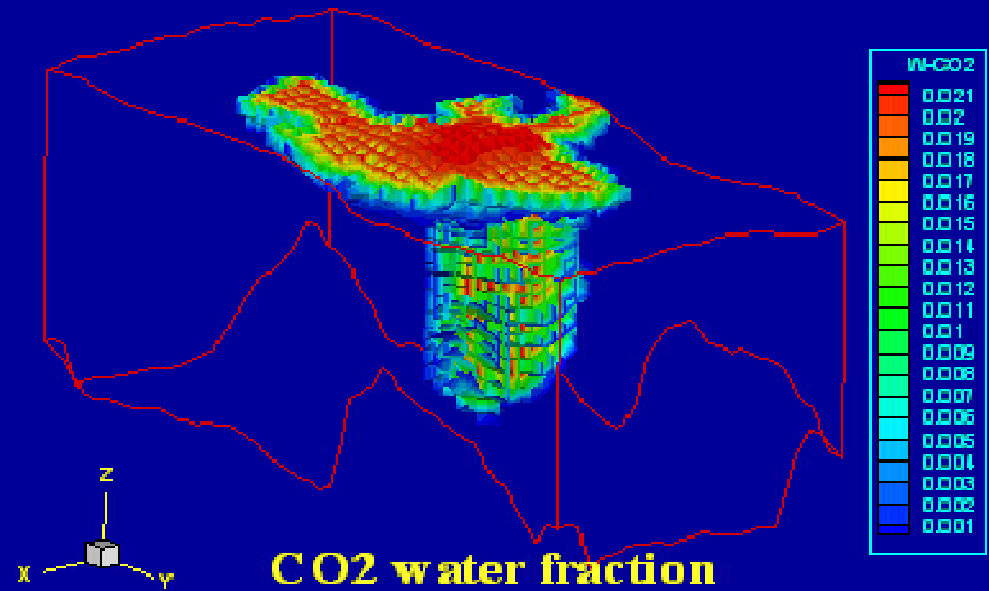
3 years



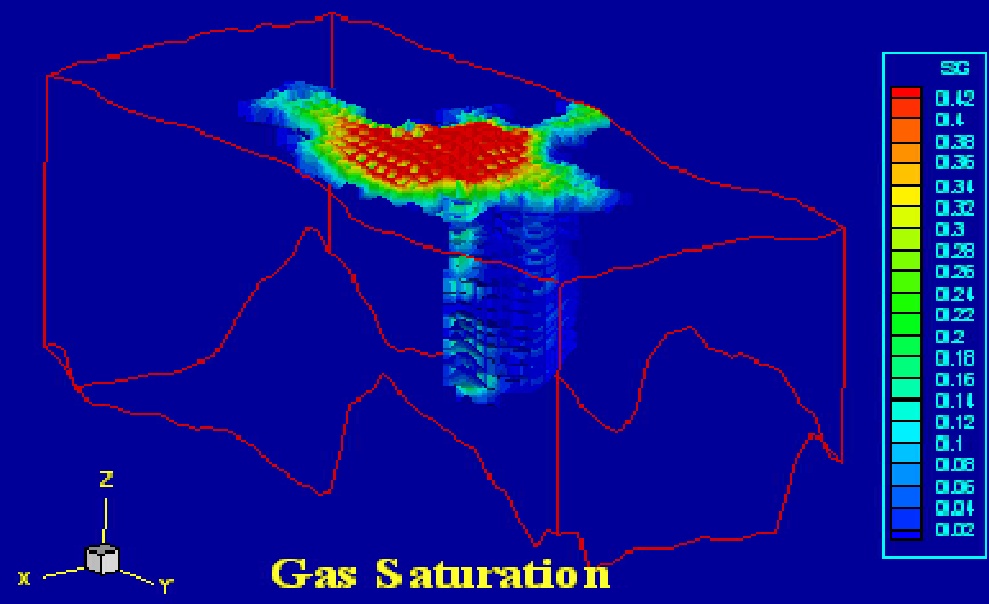


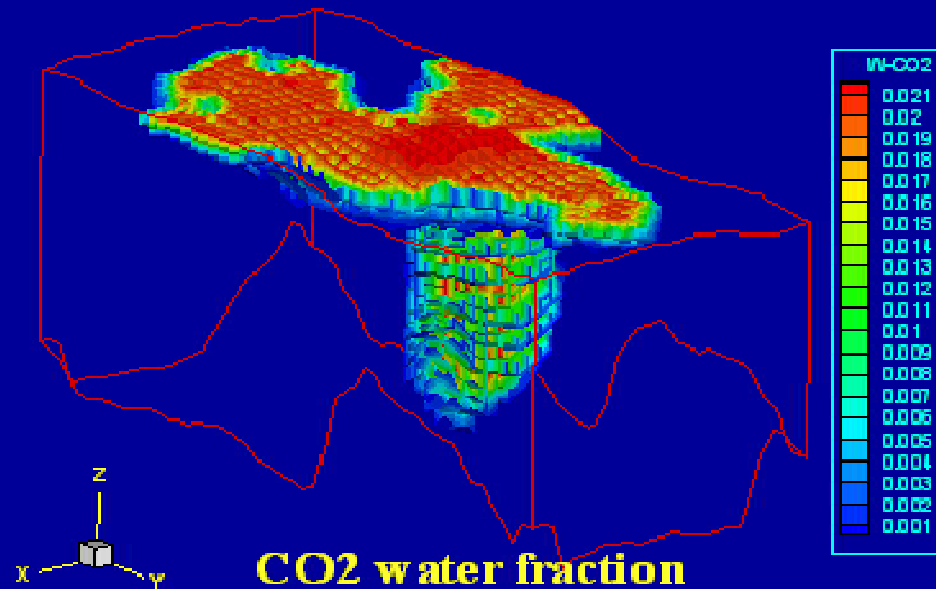
7 years





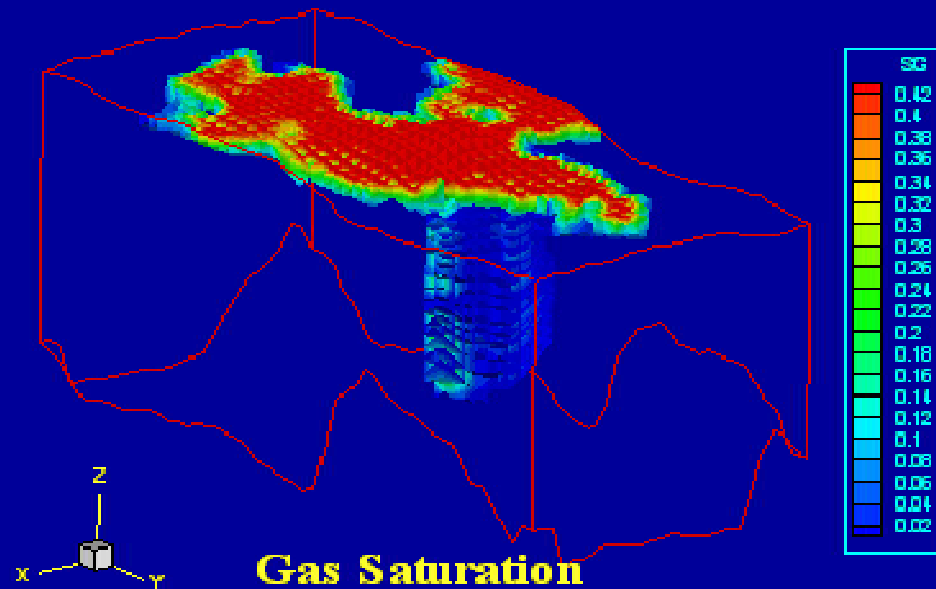
10 years



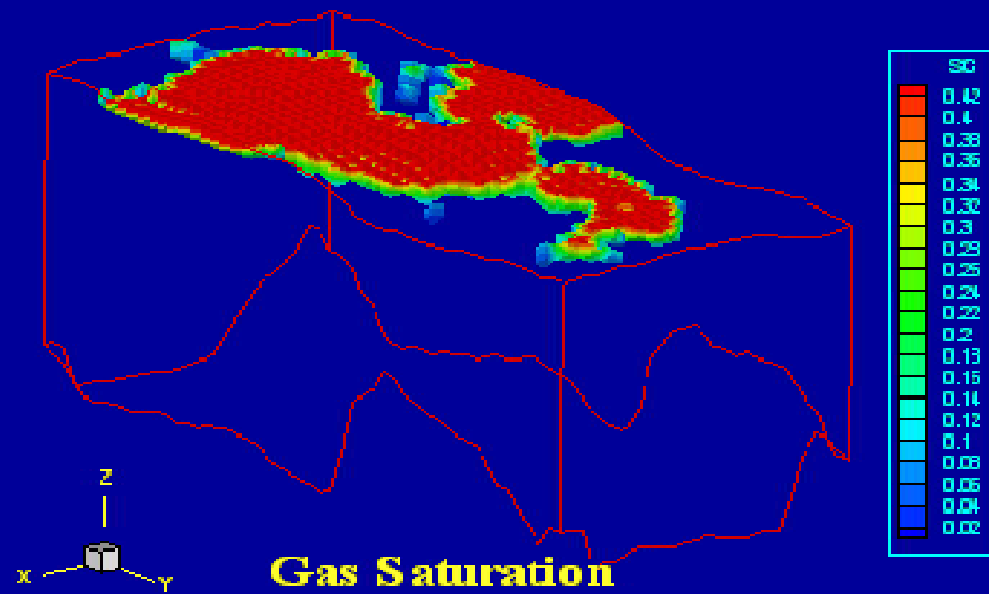
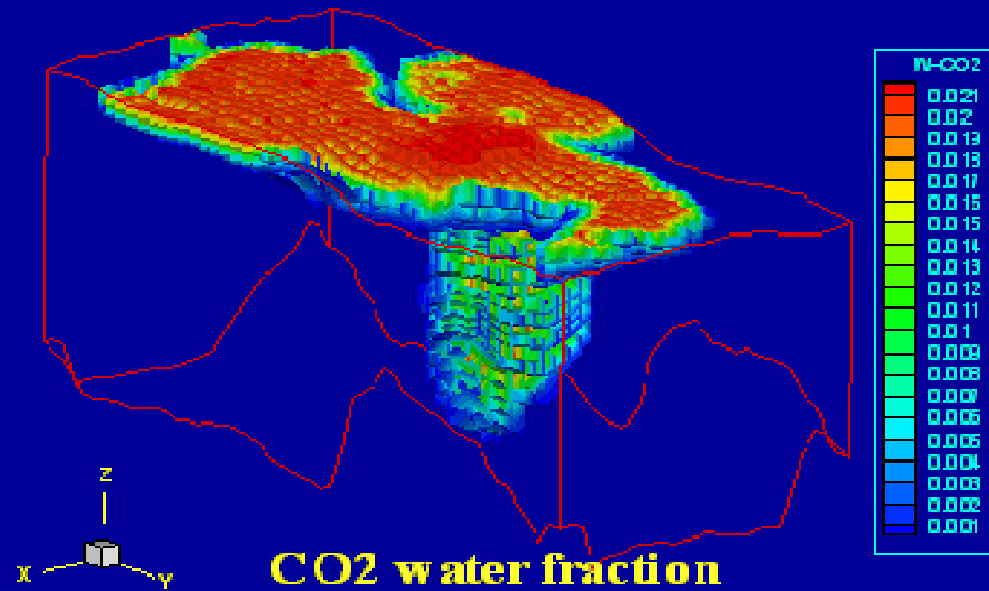


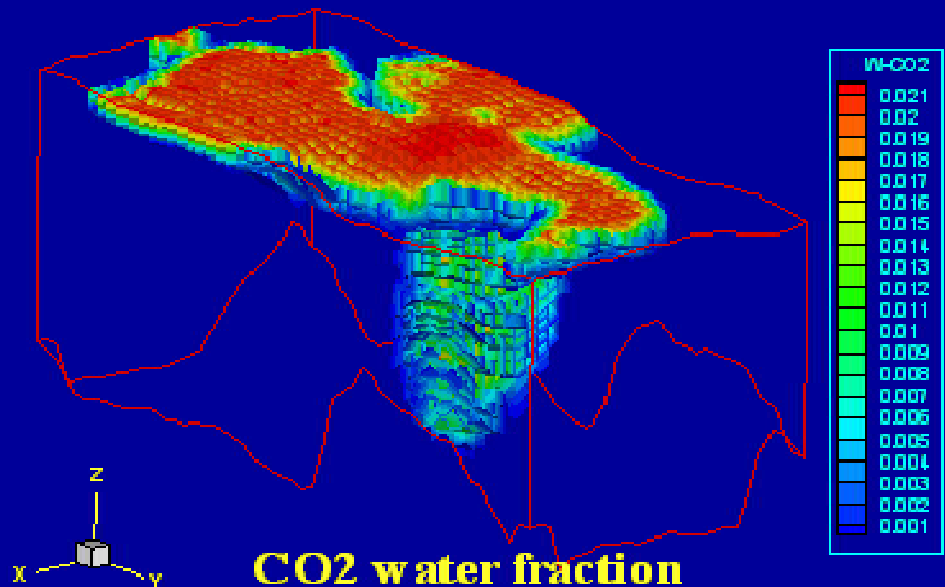
CO2 water fraction

20 years



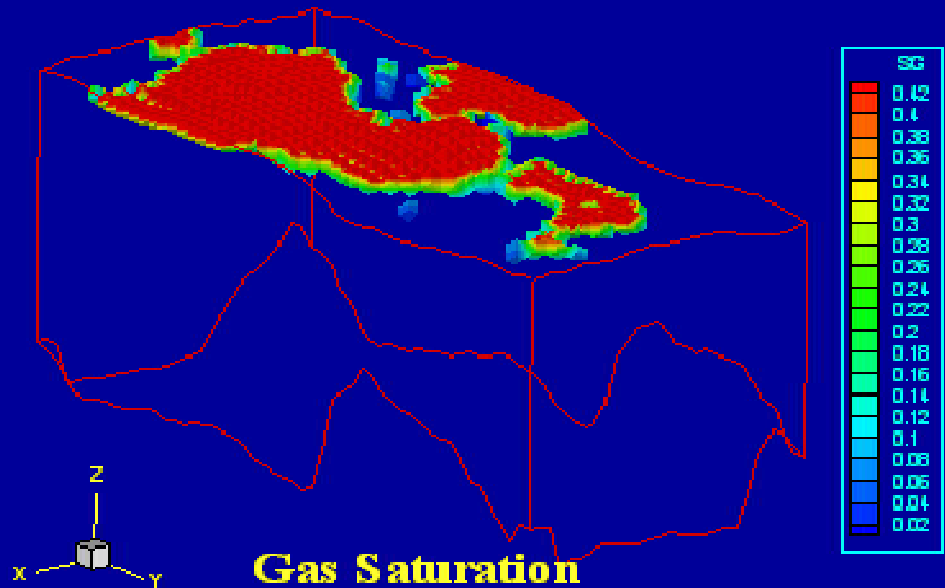
Gas Saturation



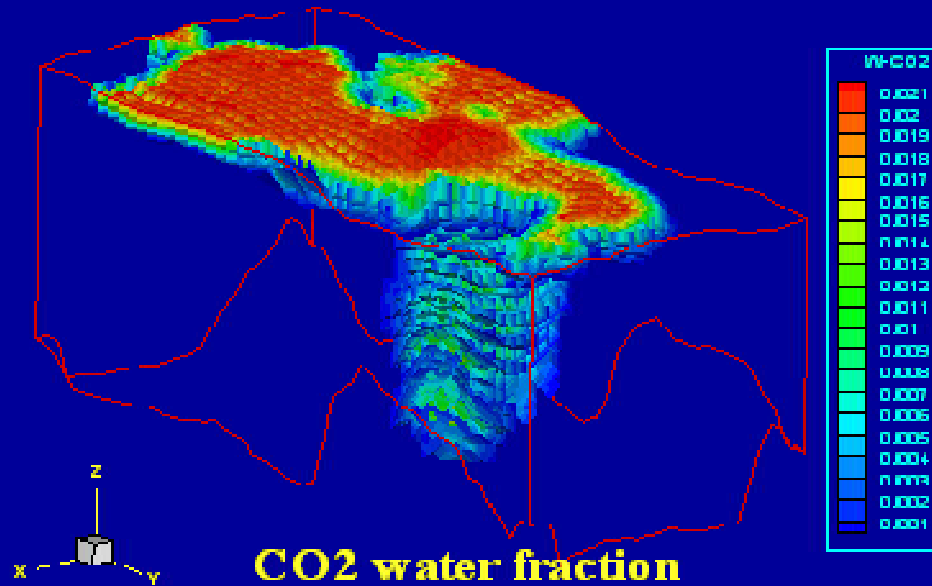


CO2 water fraction

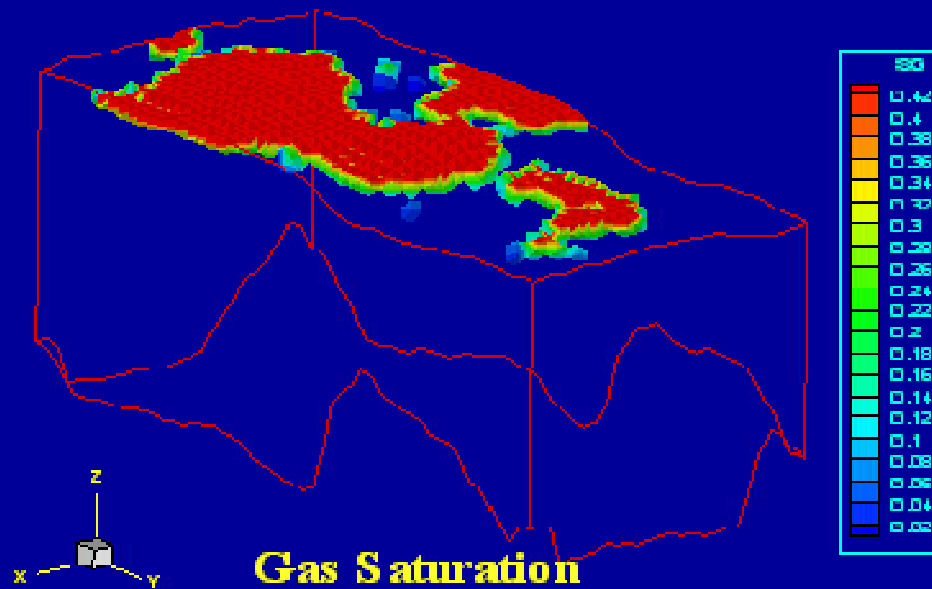
50 years

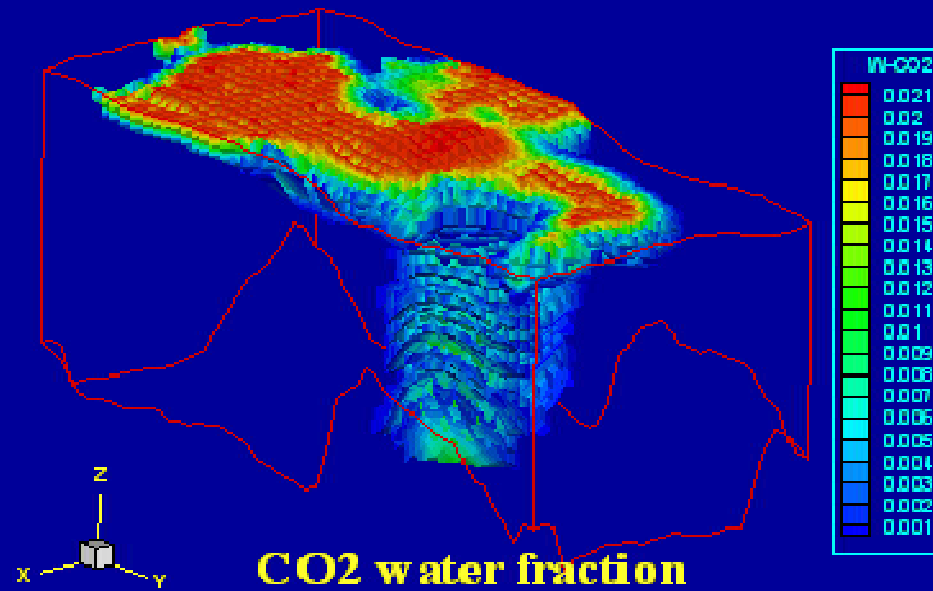


Gas Saturation

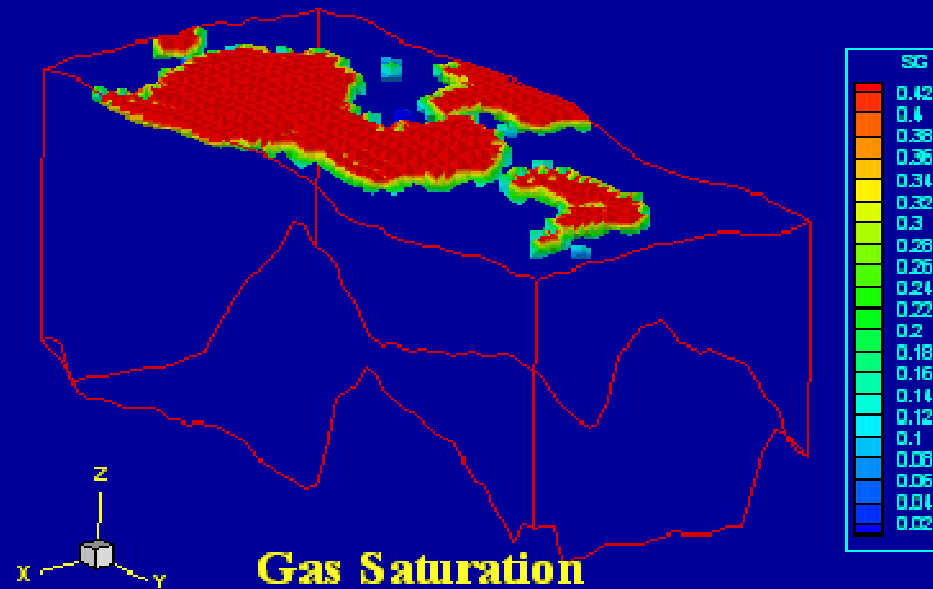


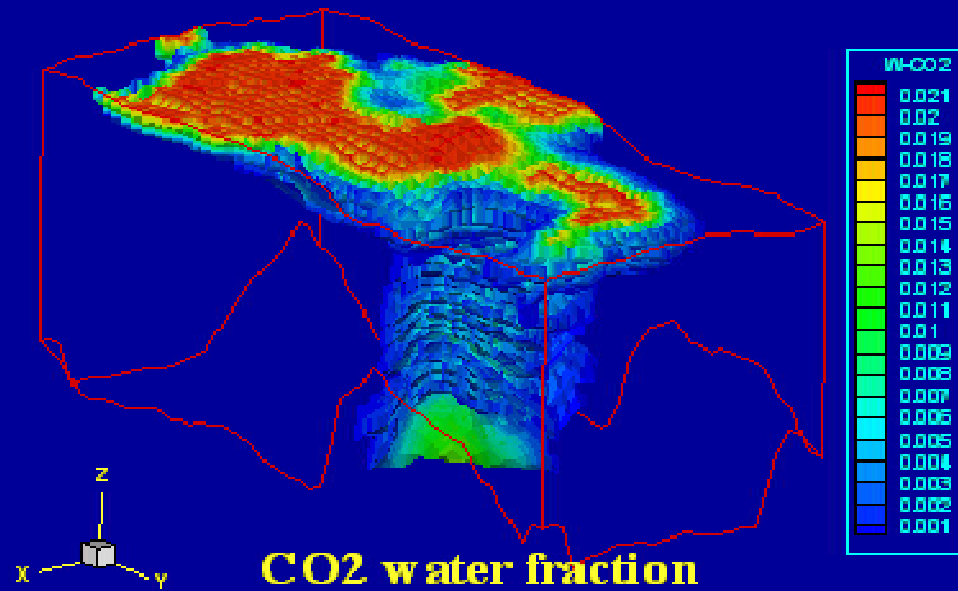
75 years



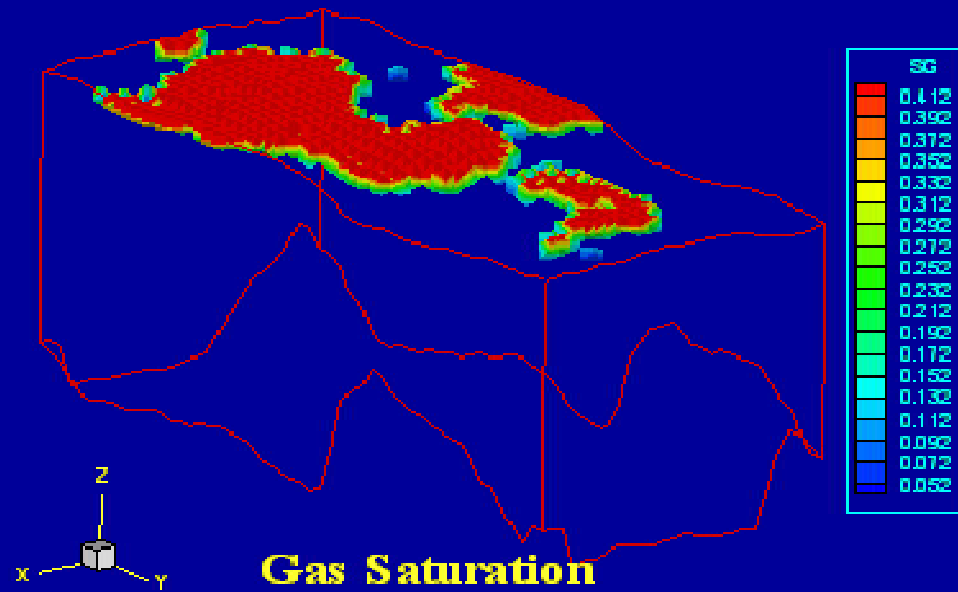


475 years



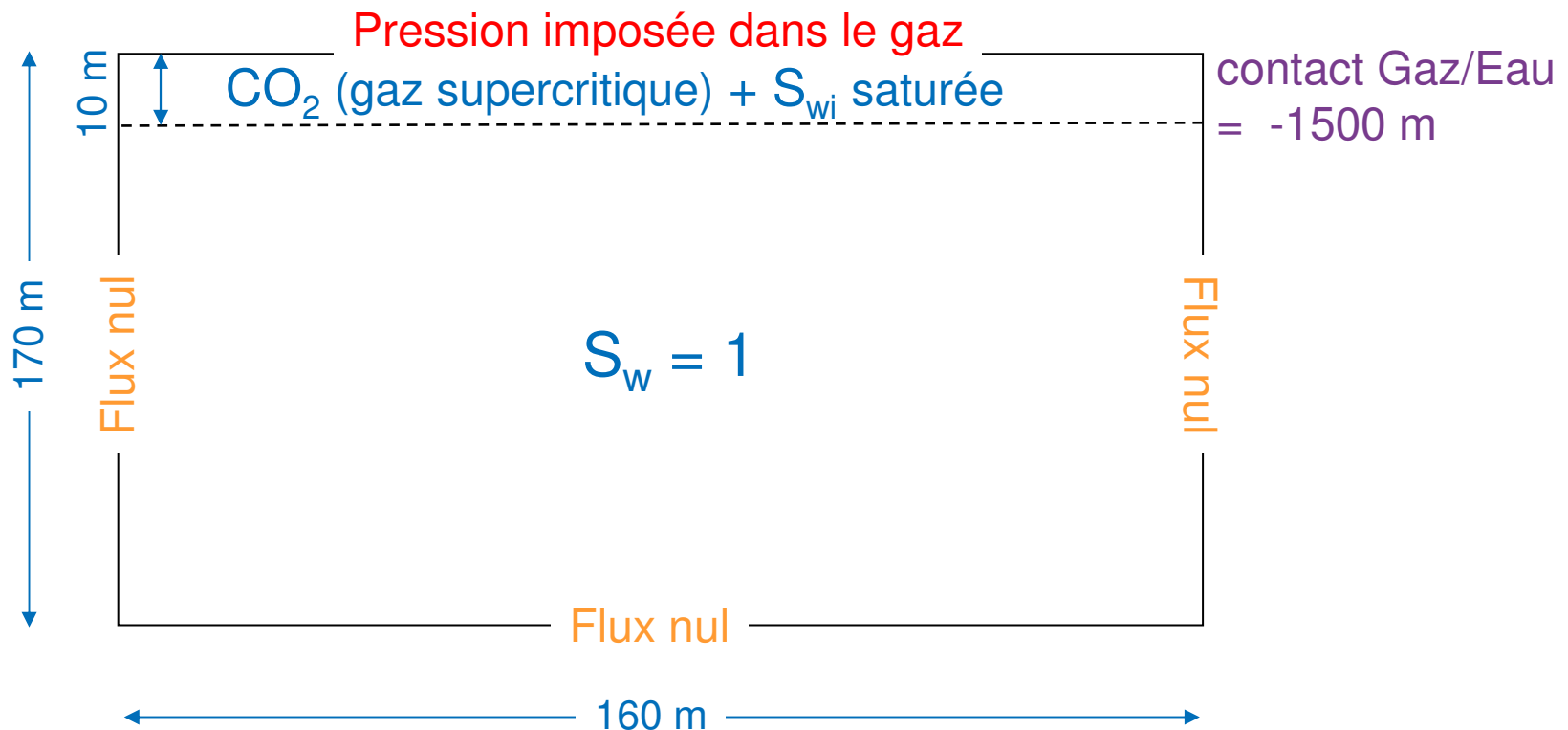


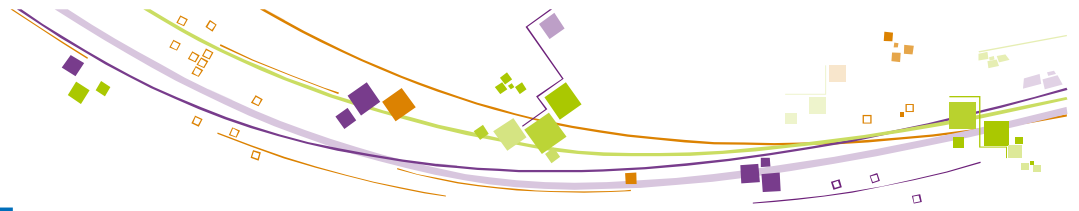
975 years





Cas Test 2D en $XZ = f(K_{mD}, D_{m^2/s})$

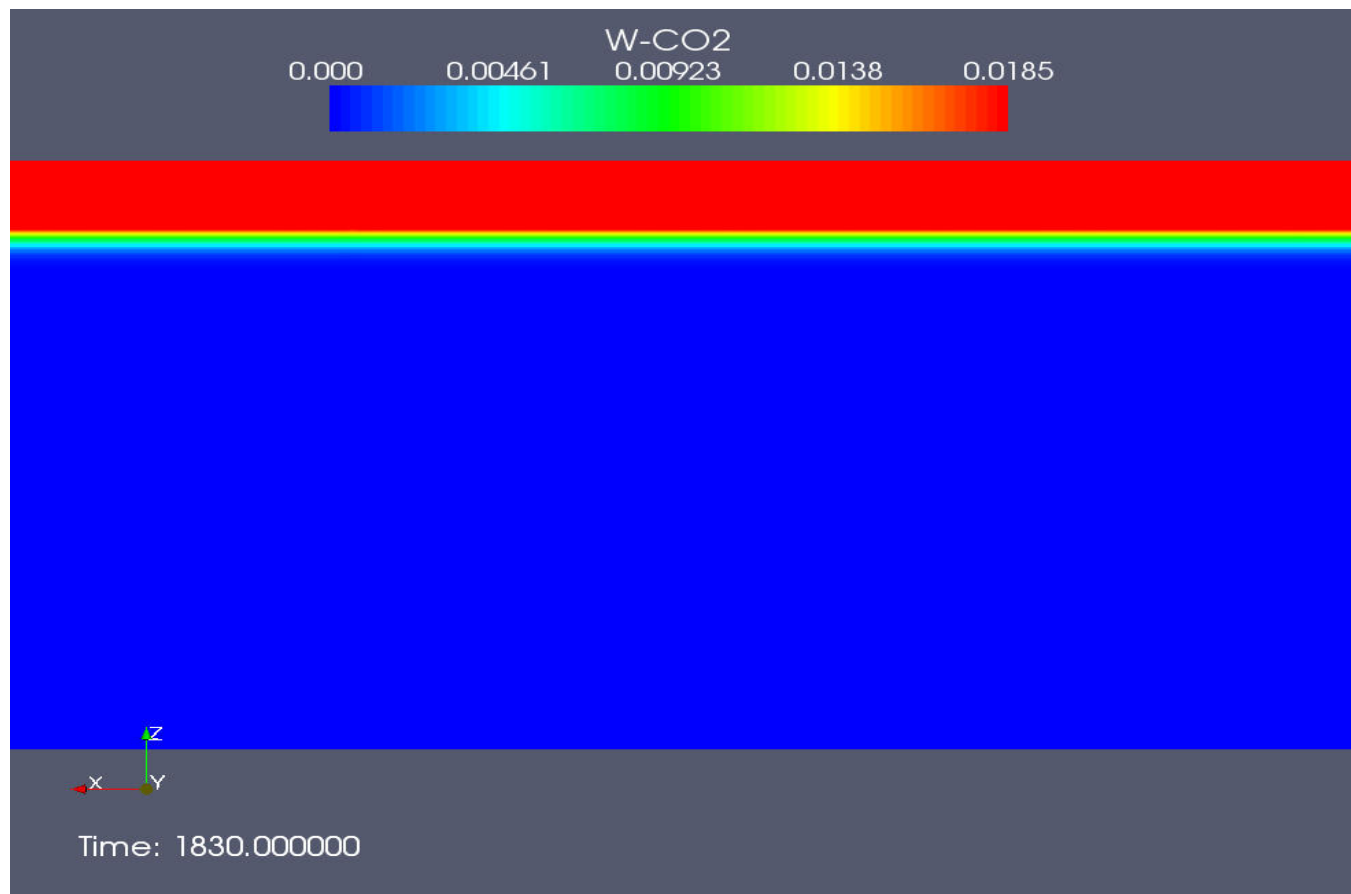


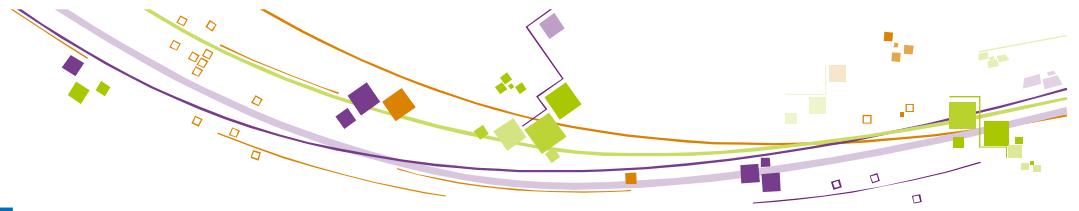


Cas Test 2D en XZ

$K = 200 \text{ mD}$ $D = 10^{-8} \text{ m}^2/\text{s}$

$t = 5 \text{ ans}$

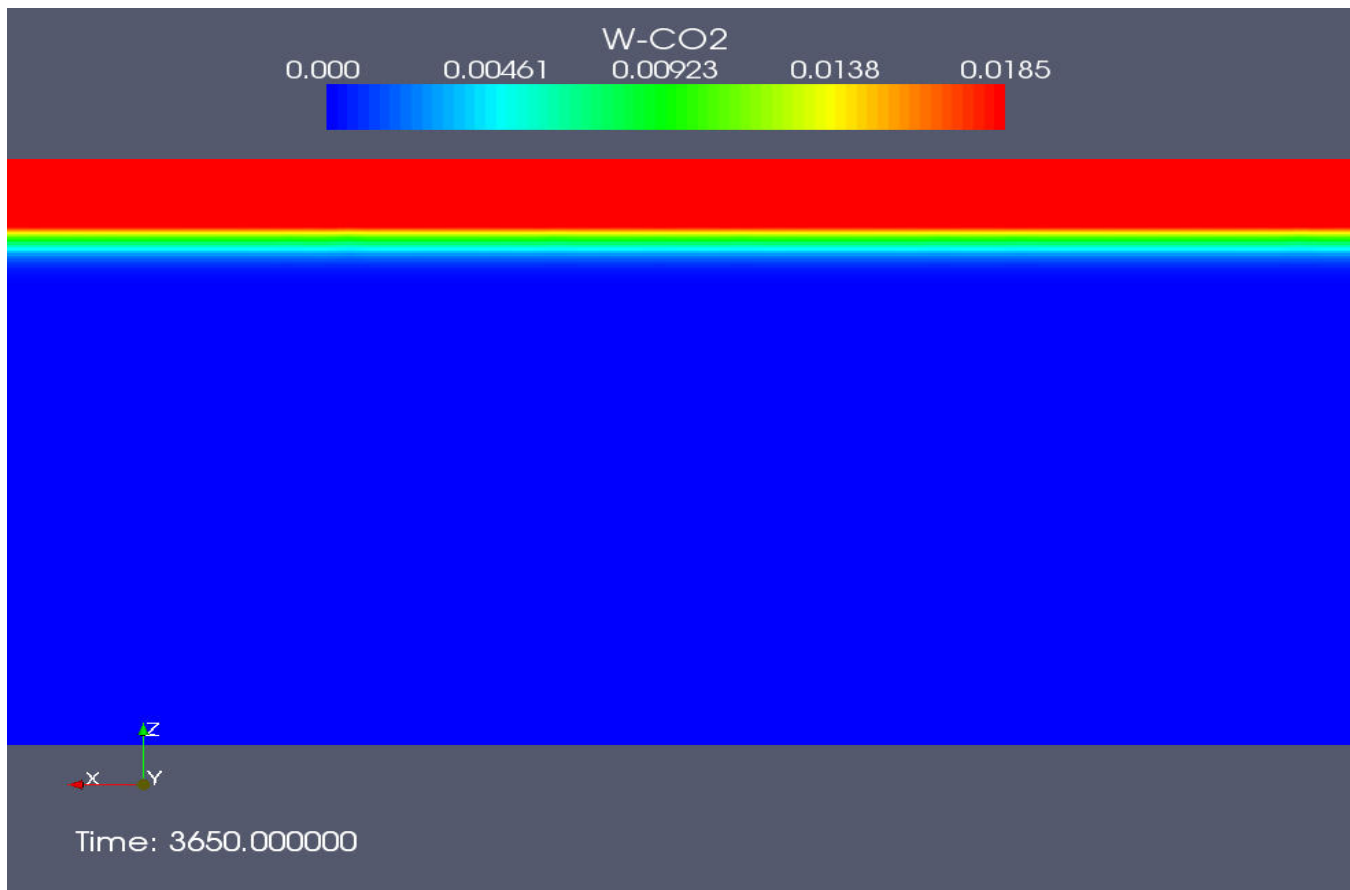


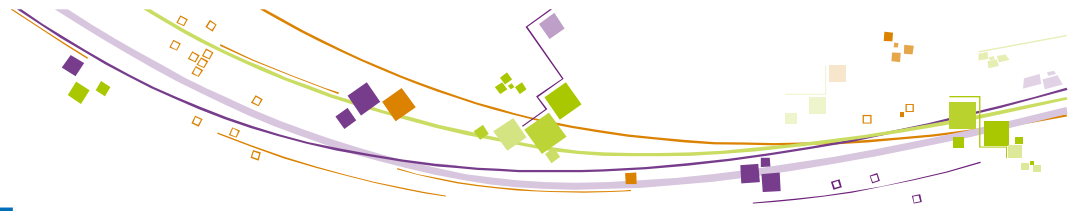


Cas Test 2D en XZ

$K = 200 \text{ mD}$ $D = 10^{-8} \text{ m}^2/\text{s}$

$t = 10 \text{ ans}$

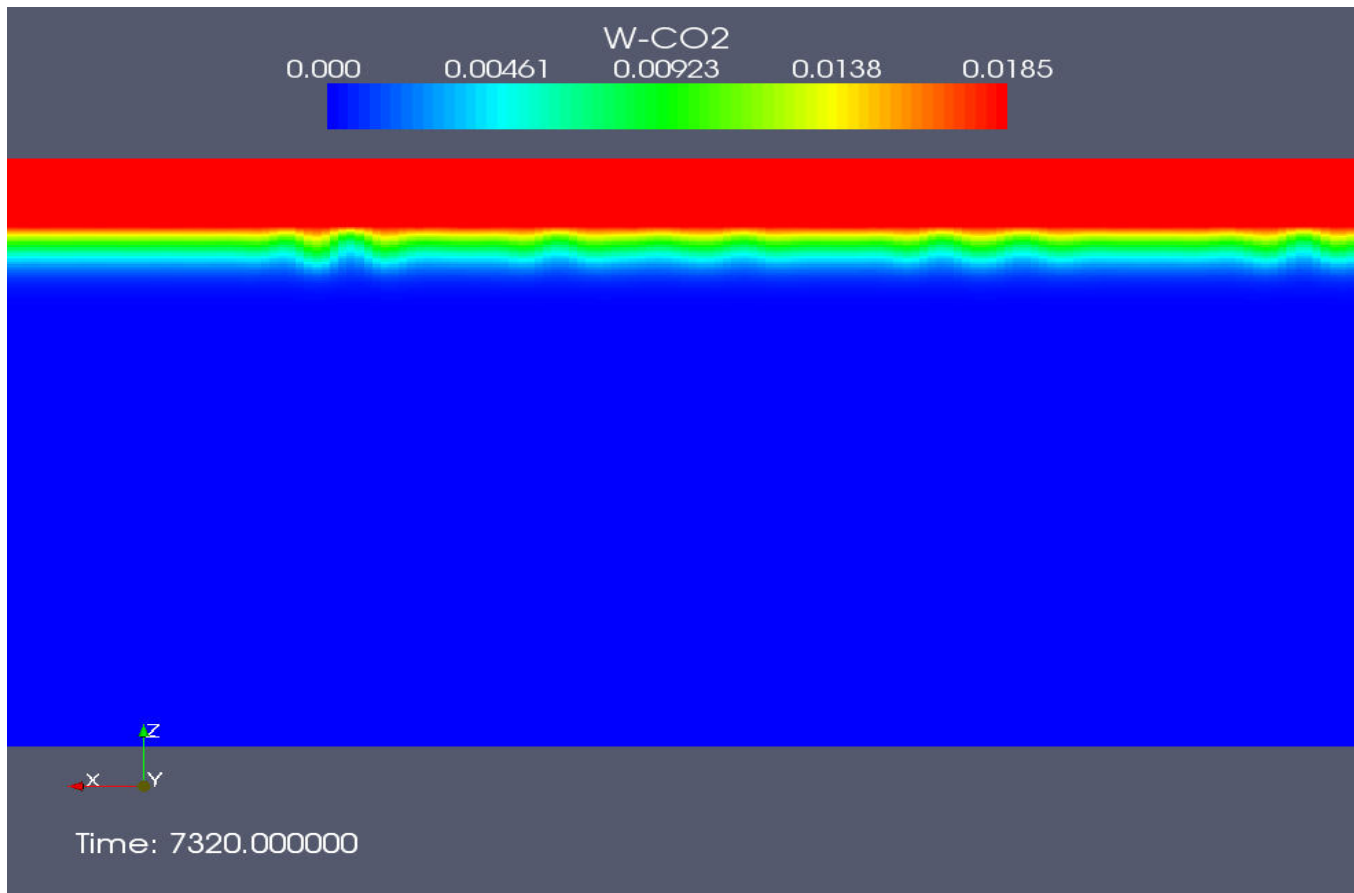


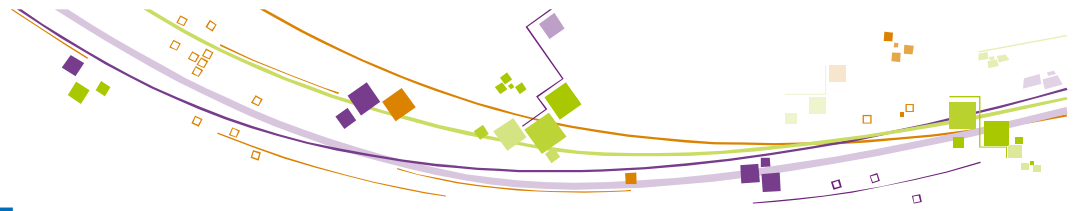


Cas Test 2D en XZ

$K = 200 \text{ mD}$ $D = 10^{-8} \text{ m}^2/\text{s}$

$t = 20 \text{ ans}$

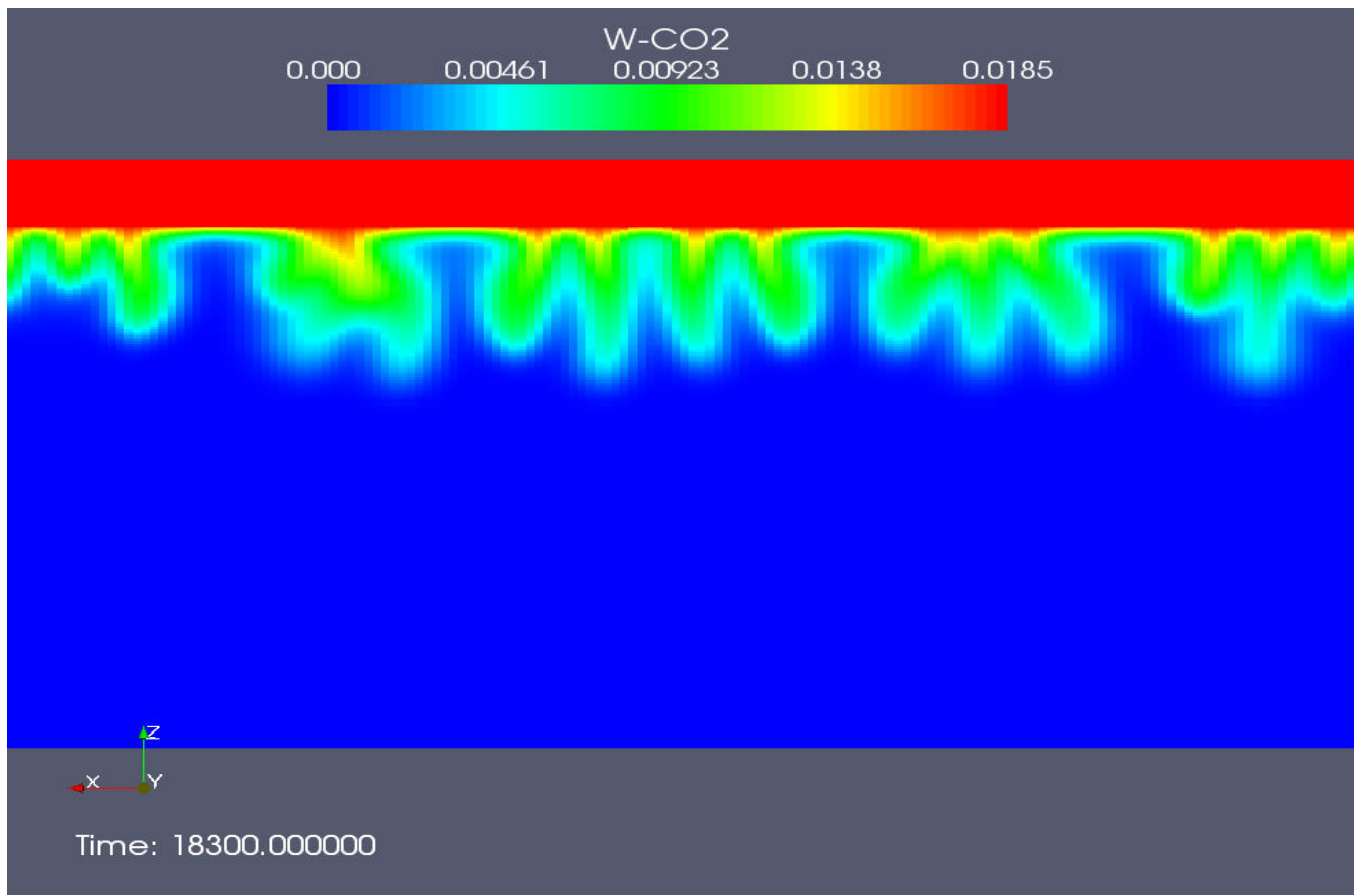


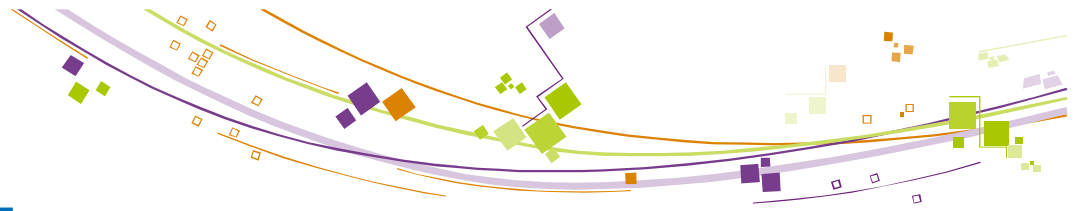


Cas Test 2D en XZ

$K = 200 \text{ mD}$ $D = 10^{-8} \text{ m}^2/\text{s}$

$t = 50 \text{ ans}$

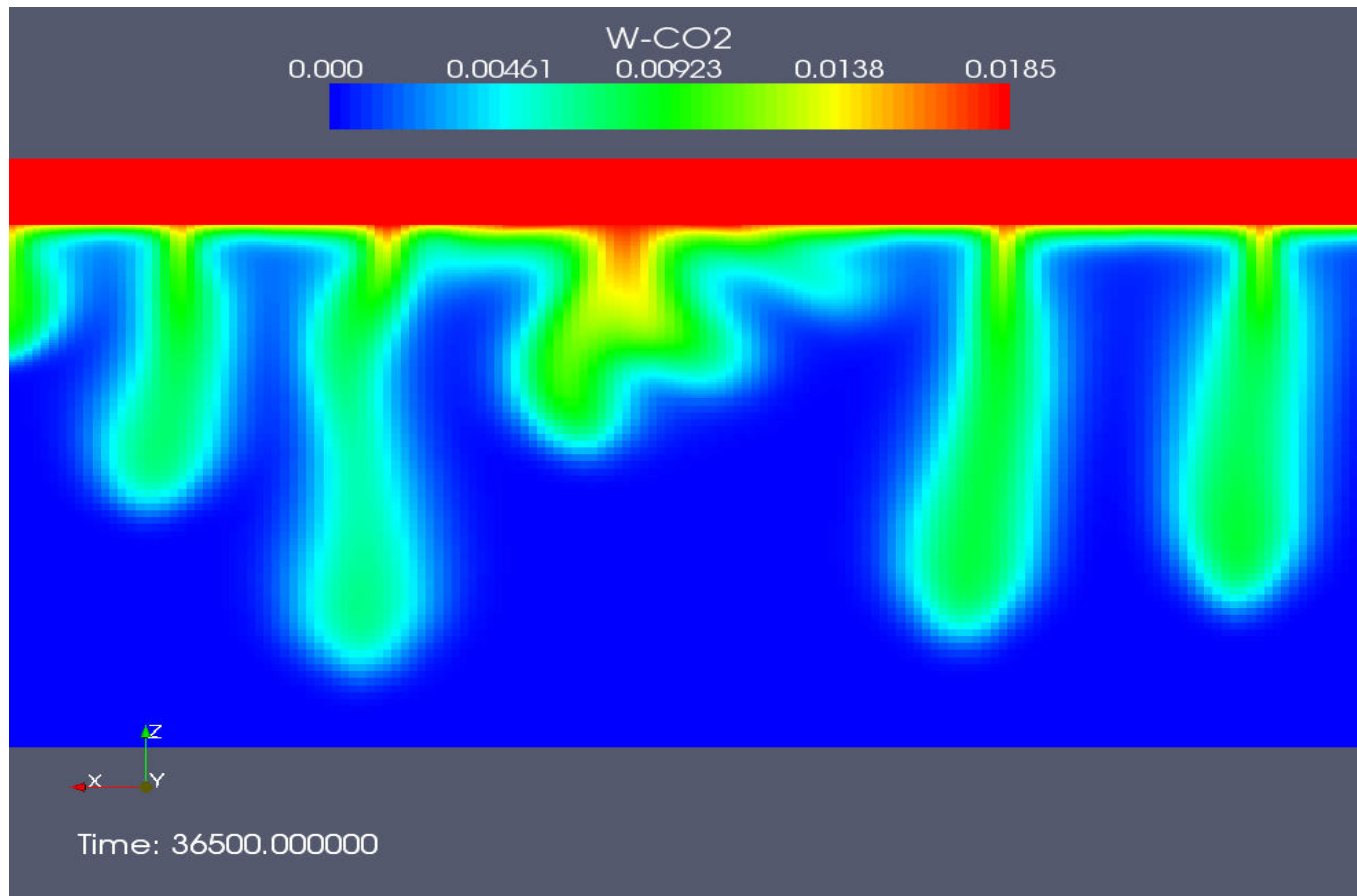


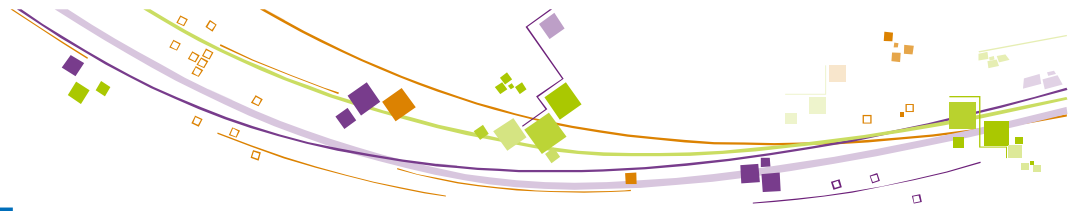


Cas Test 2D en XZ

$K = 200 \text{ mD}$ $D = 10^{-8} \text{ m}^2/\text{s}$

$t = 100 \text{ ans}$

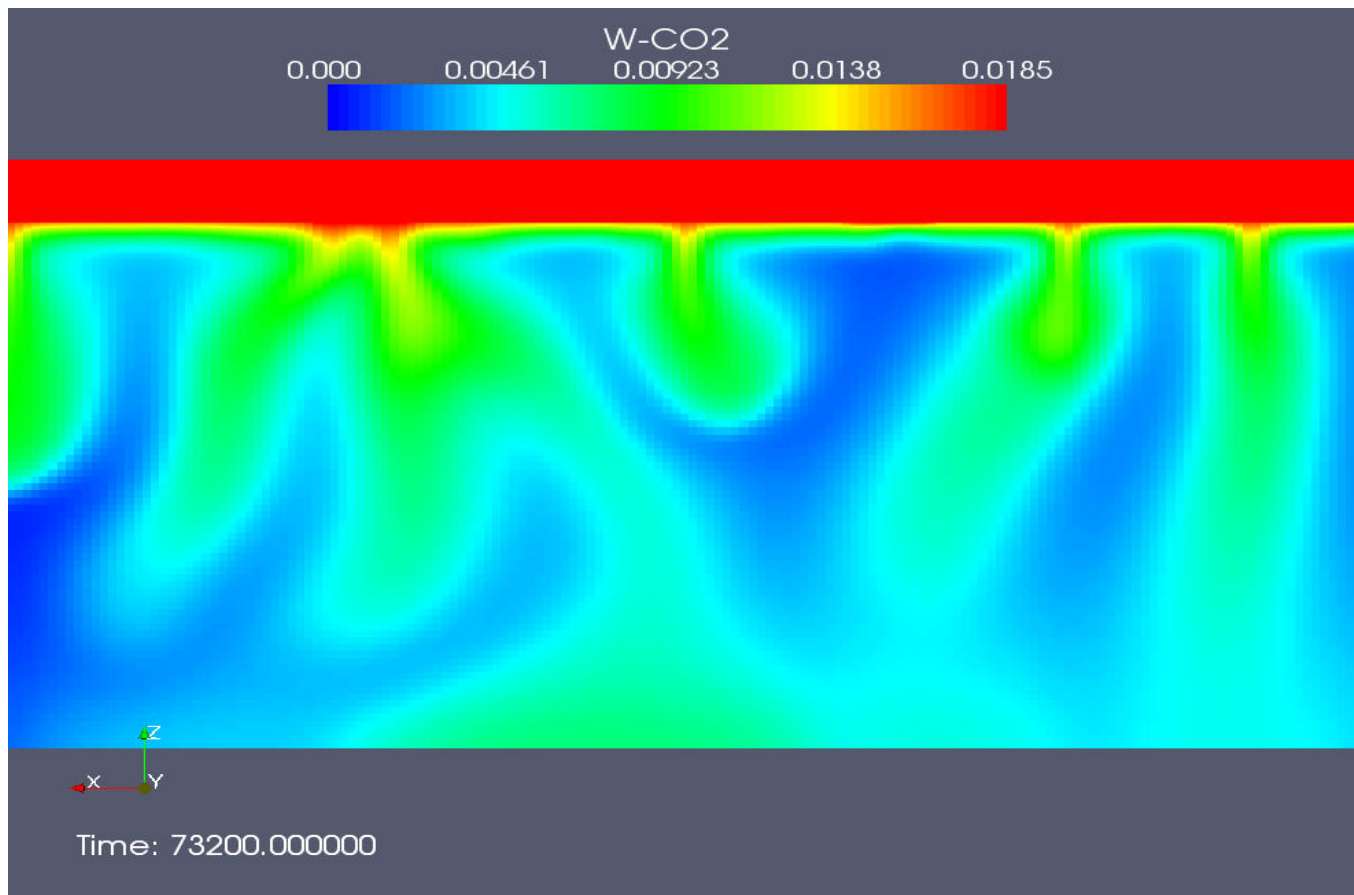


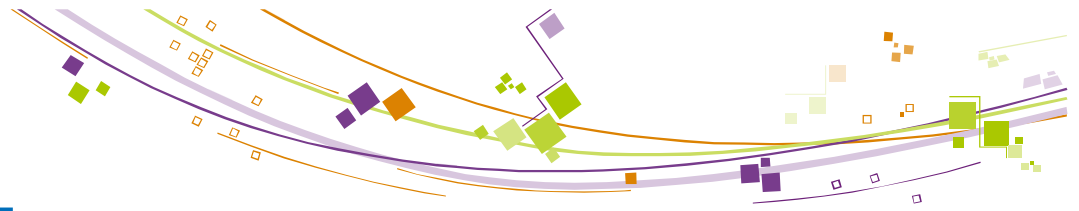


Cas Test 2D en XZ

$K = 200 \text{ mD}$ $D = 10^{-8} \text{ m}^2/\text{s}$

$t = 200 \text{ ans}$

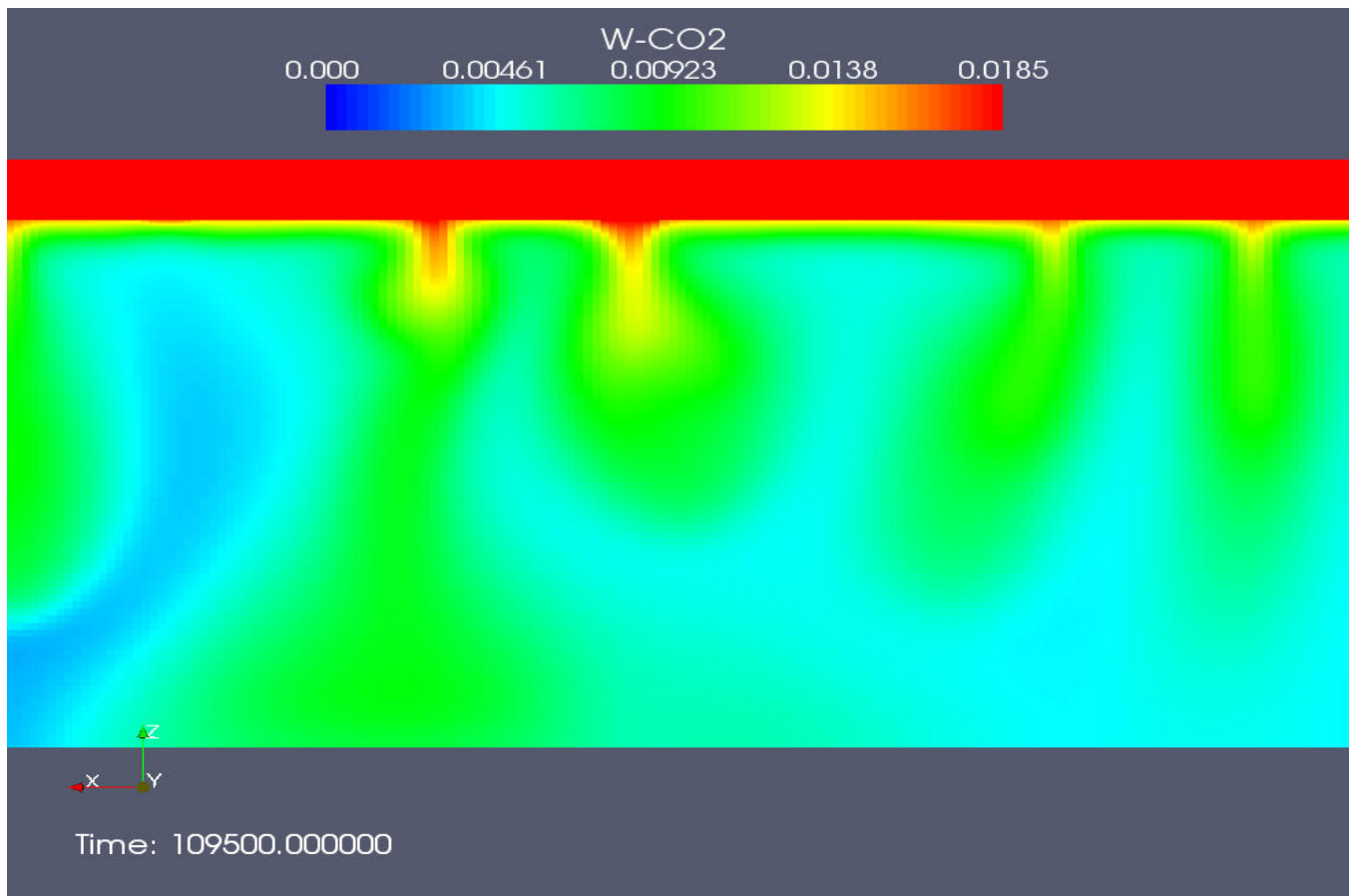


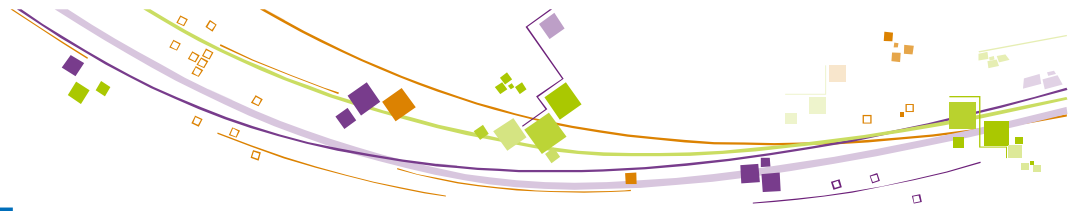


Cas Test 2D en XZ

$K = 200 \text{ mD}$ $D = 10^{-8} \text{ m}^2/\text{s}$

$t = 300 \text{ ans}$

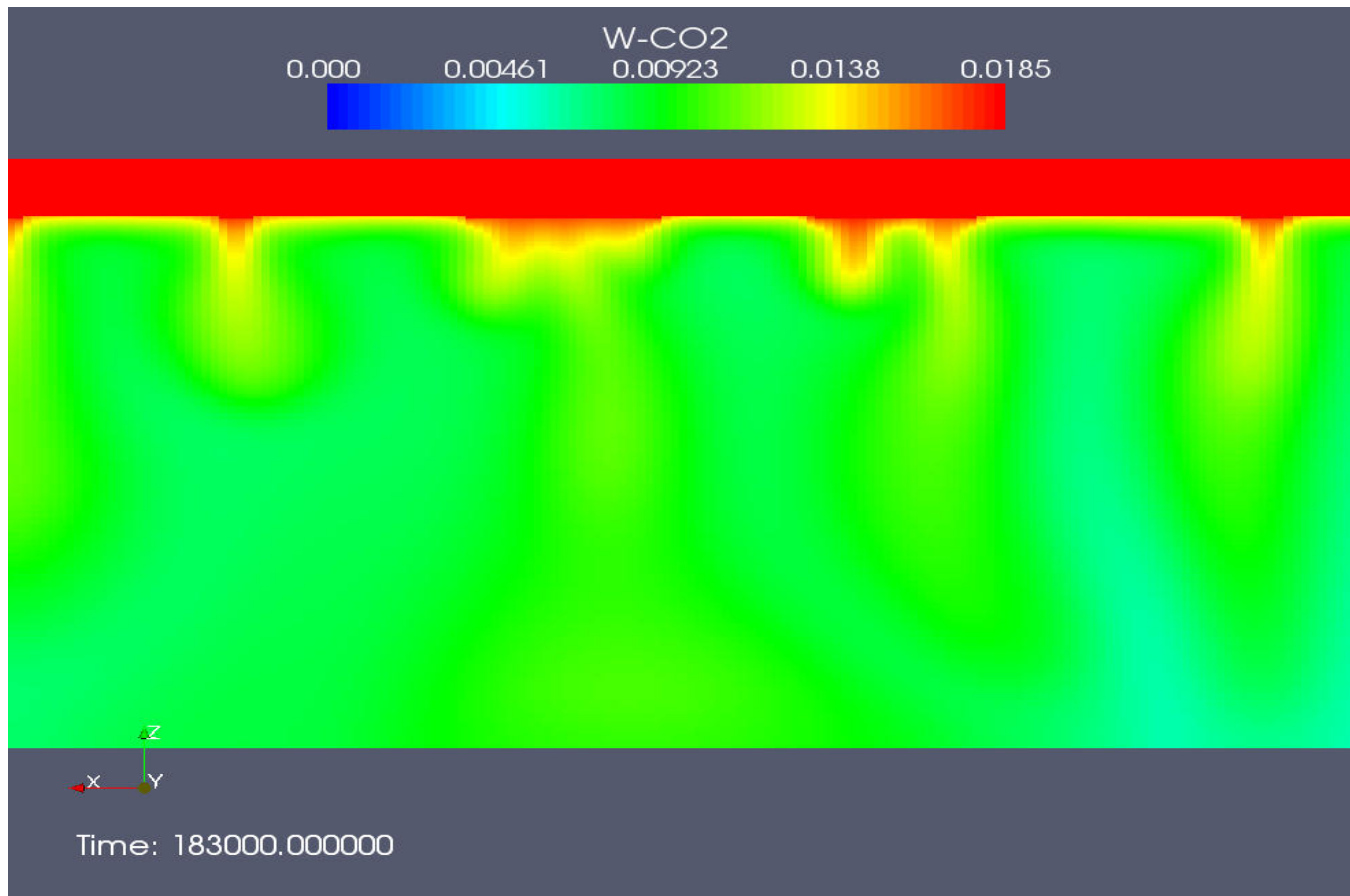




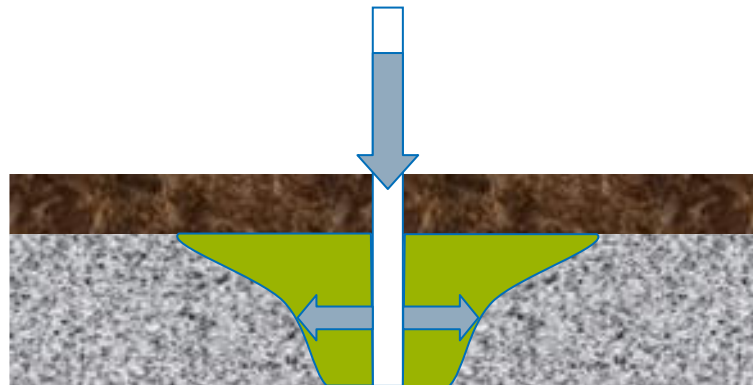
Cas Test 2D en XZ

$K = 200 \text{ mD}$ $D = 10^{-8} \text{ m}^2/\text{s}$

$t = 500 \text{ ans}$



Écoulements proche puits avec vaporisation de l'eau et dépôt de sel

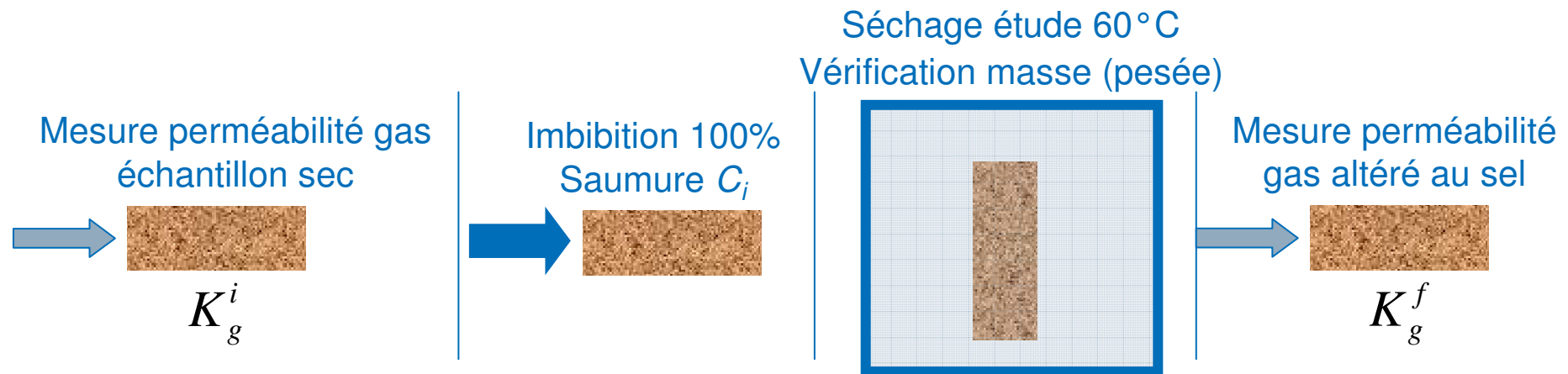


Écoulement de gaz sec => assèchement de la zone proche puits

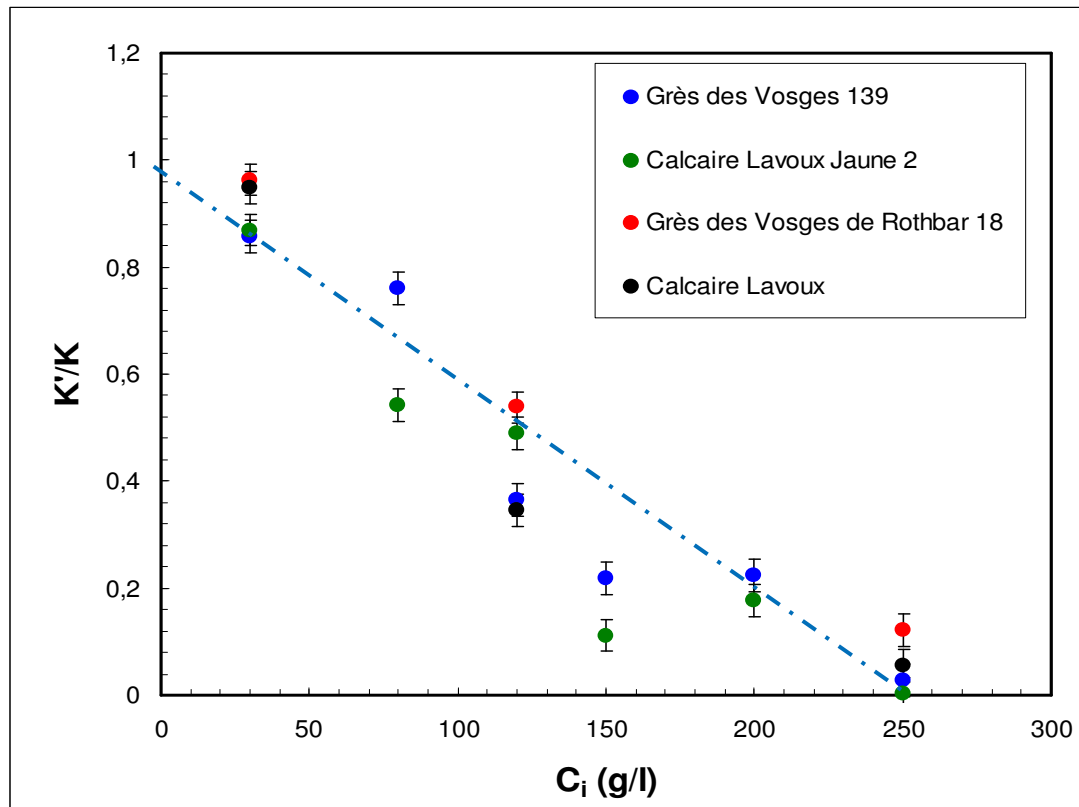
Peut-on avoir une altération de perméabilité par précipitation du sel ?



Dépôt de sel au voisinage du puits: expériences en laboratoire (Yannick Peysson IFP)



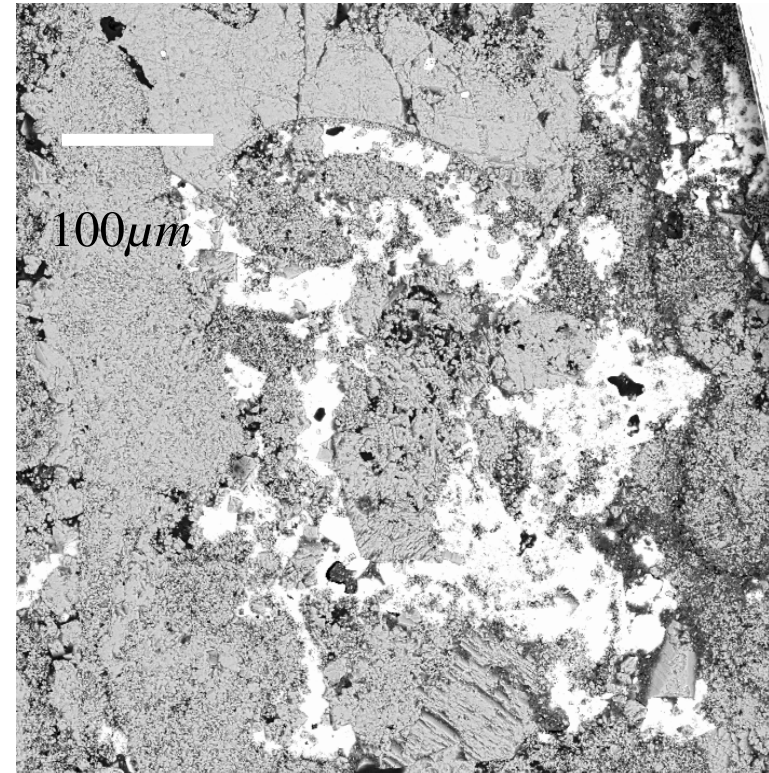
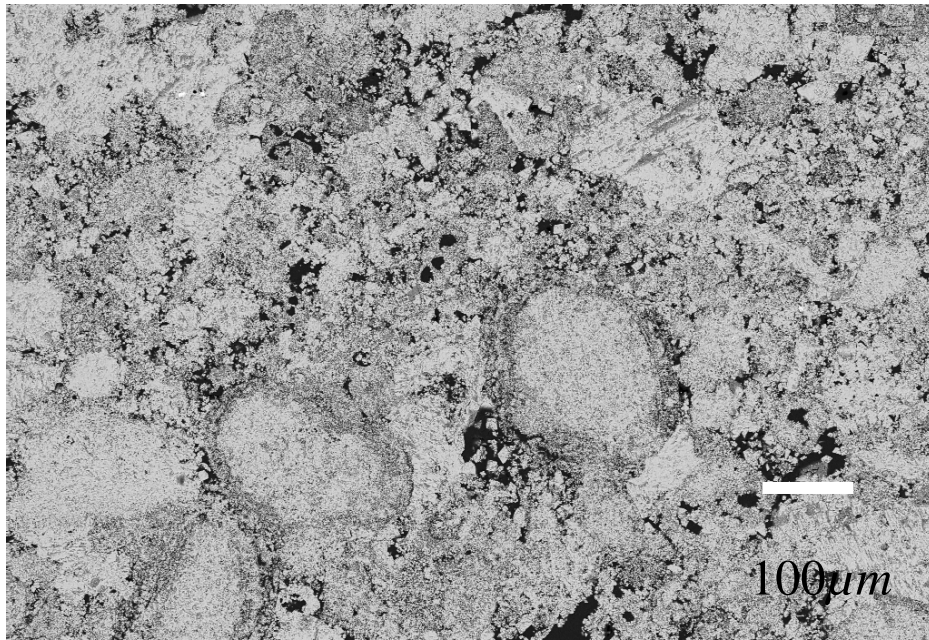
Dépôt de sel au voisinage du puits: expériences en laboratoire (Yannick Peysson IFP)



- Relativement peu dépendant du matériaux
- Relativement peu dépendant de la perméabilité initiale
- Altération à presque 100% à $C_i=250$ g/l (identique pour les 4 séries)



Calcaire de Lavoux



Porosité remplie de KCl
Pas de porosité du sel

Calcaire Lavoux
 $\text{Ø}=24,6\%$
 $K_{gi}=3,83 \text{ mD}$

Modèle triphasique w-g-m à trois composants H₂O, CO₂, Sel

$$\left\{ \begin{array}{l} \partial_t \phi \left(\rho^w S^w C_{H_2O}^w + \rho^g S^g C_{H_2O}^g \right) + \text{div} \left(C_{H_2O}^w \rho^w \mathbf{V}^w + C_{H_2O}^g \rho^g \mathbf{V}^g \right) \\ \quad + \text{div} \left(-\phi \rho^w S^w D_{sel}^w \nabla C_{H_2O}^w \right) = 0, \\ \\ \partial_t \phi \left(\rho^w S^w C_{Sel}^w + \rho^m S^m \right) + \text{div} \left(C_{Sel}^w \rho^w \mathbf{V}^w \right) \\ \quad + \text{div} \left(-\phi \rho^w S^w D_{sel}^w \nabla C_{Sel}^w \right) = 0, \\ \\ \partial_t \phi \left(\rho^g S^g C_{CO_2}^g \right) + \text{div} \left(C_{CO_2}^g \rho^g \mathbf{V}^g \right) = 0 \end{array} \right.$$

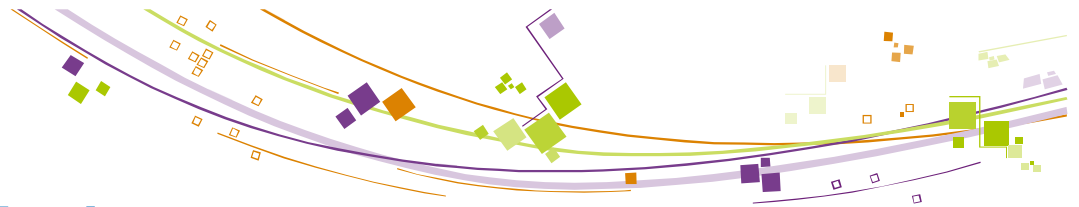
$$\left\{ \begin{array}{ll} S^w + S^g + S^m = 1, & \\ C_{H_2O}^w + C_{Sel}^w = 1, & \text{si phase w présente} \\ C_{H_2O}^g + C_{CO_2}^g = 1, & \text{si phase g présente} \\ C_{H_2O}^g = K_{H_2O}^{gw} C_{H_2O}^w, & \text{si phases w et g présentes,} \\ C_{Sel}^w = K_{Sel}, & \text{si phases w et m présentes.} \end{array} \right.$$

Modèle triphasique w-g-m à trois composants H₂O, CO₂, Sel

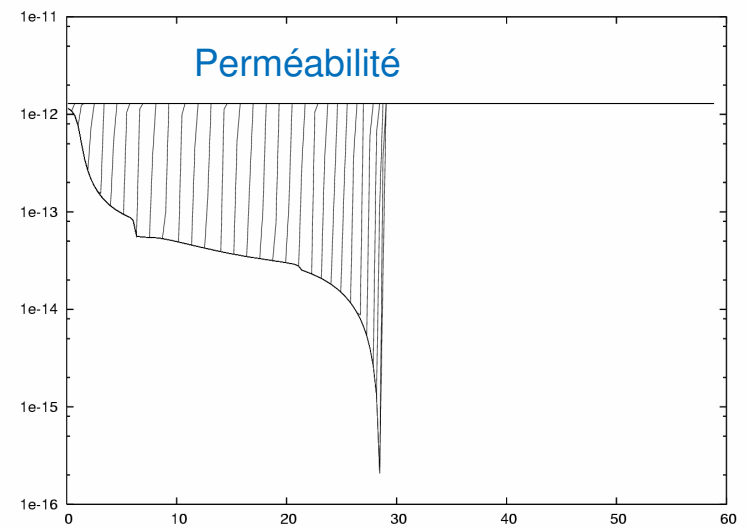
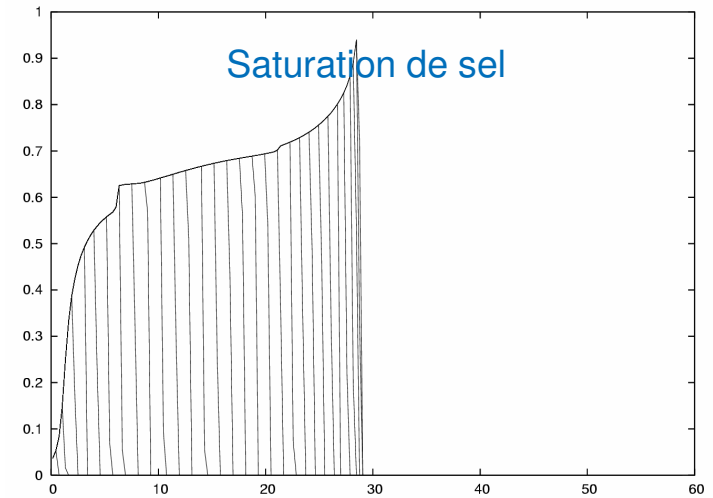
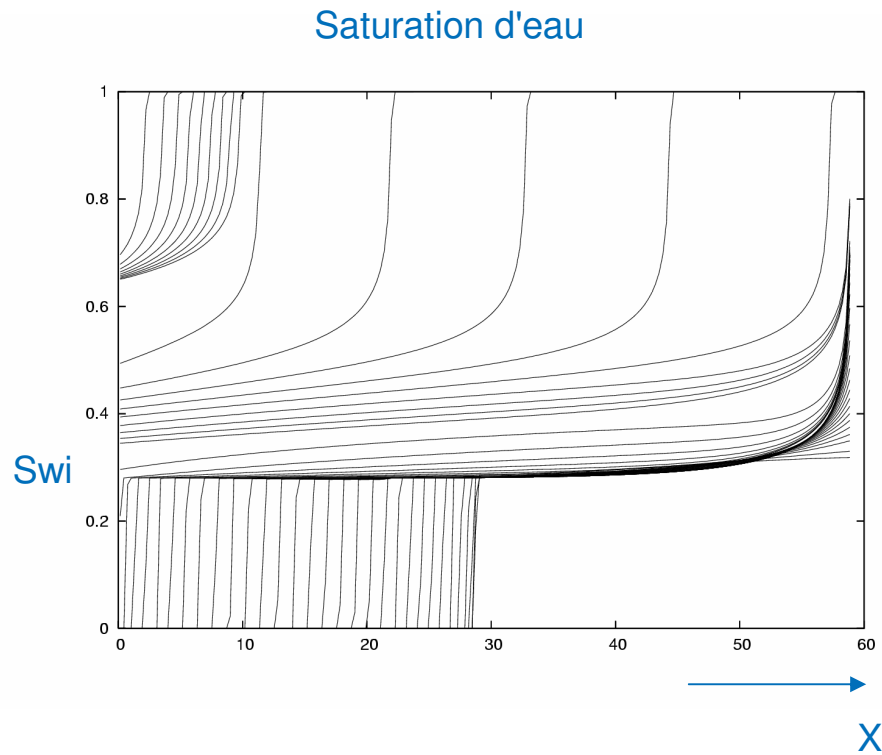
- Détermination des phases présentes par flash à P,Z donnés
- Combinatoire
 - Flash étendu triphasique w-g-m
 - Flash étendus diphasiques w-g, w-m, g-m

Flash étendu triphasique à P,Z donnés → fractions massiques des phases et compositions des phases

$$\left\{ \begin{array}{l} Z_{H_2O} = \theta^g C_{H_2O}^g + \theta^w C_{H_2O}^w, \\ Z_{CO_2} = \theta^g C_{CO_2}^g, \\ Z_{sel} = \theta^w C_{Sel}^w + \theta^m, \\ \theta^g + \theta^w + \theta^m = 1, \\ C_{H_2O}^w + C_{Sel}^w = 1, \\ C_{H_2O}^g + C_{CO_2}^g = 1, \\ C_{H_2O}^g = K_{H_2O}^{gw} C_{H_2O}^w, \\ C_{Sel}^w = K_{Sel}, \\ C_{H_2O}^w \geq 0, C_{Sel}^w \geq 0, \\ C_{H_2O}^g \geq 0, C_{CO_2}^g \geq 0. \end{array} \right.$$



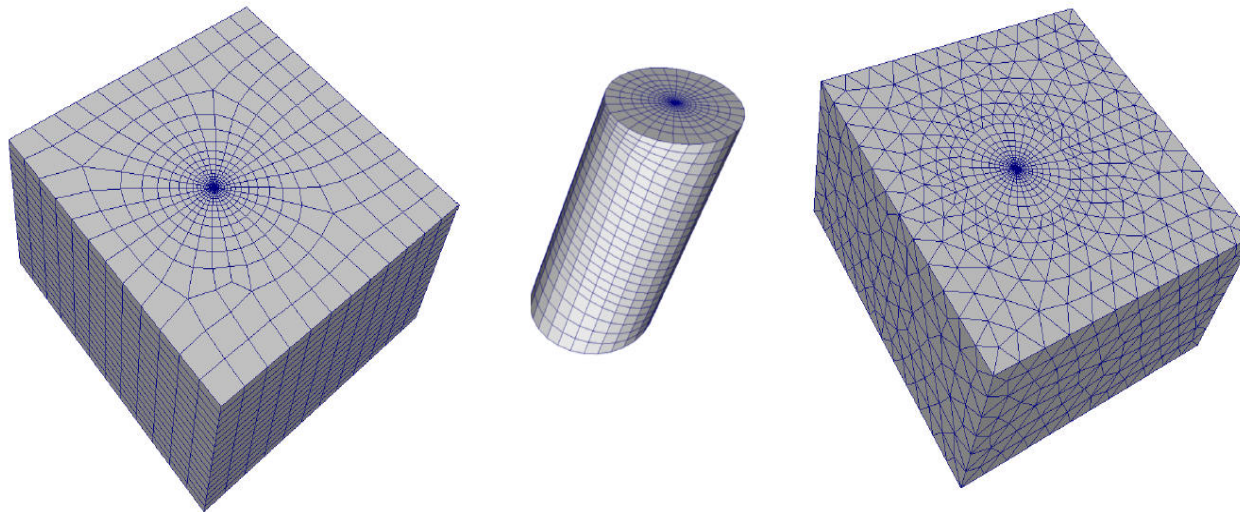
Assèchement et dépôt de sel



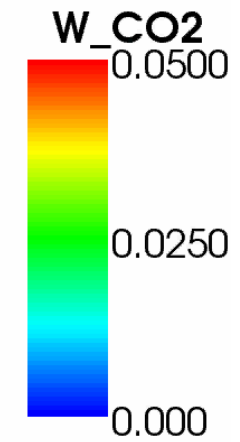
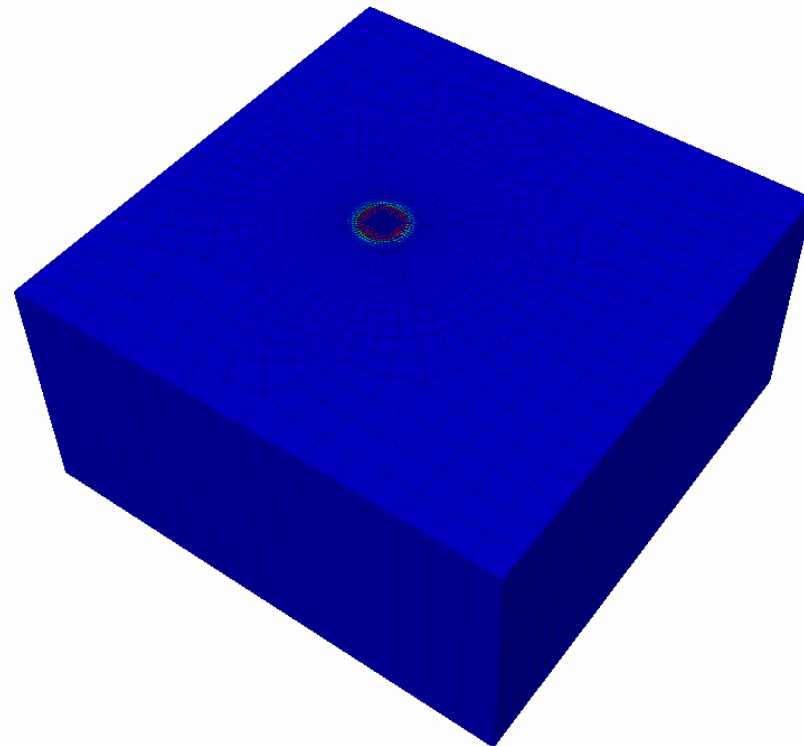


Modèle proche puits 3D

- *dimension* : $L_x \times L_y \times L_z = 30\text{m} \times 30\text{m} \times 15\text{m}$
- *rayon zone radiale* : $R_d = 5\text{m}$
- *rayon puits* : $r_w = 0.1\text{m}$
- *inclinaison puits* : 20° par rapport à l'axe z



Modèle proche puits 3D



Modèles Polyphasiques Compositionnels

Phases: $\alpha = 1, \dots, N_p$ (eau, huile, gaz, ...)

Composants $i=1, \dots, N_c$ (H_2O , HCs, CO_2 , ...)

Inconnues

$$P, S_\alpha = \frac{Vol_\alpha}{Vol_{Pore}}, C_i^\alpha = \frac{m_i^\alpha}{m^\alpha}$$

Loi de Darcy
polyphasique

$$\left\{ \begin{array}{l} \mathbf{V}_\alpha = -\frac{k_{r,\alpha}}{\mu_\alpha} K (\nabla (P + P_{c,\alpha}) + \rho_\alpha \vec{g}) \\ \partial_t \left(\phi \sum_\alpha \rho_\alpha C_i^\alpha S_\alpha \right) + \text{div} \left(\sum_\alpha \rho_\alpha C_i^\alpha \mathbf{V}_\alpha \right) = Q_i \\ \sum_\alpha S_\alpha = 1 \end{array} \right.$$

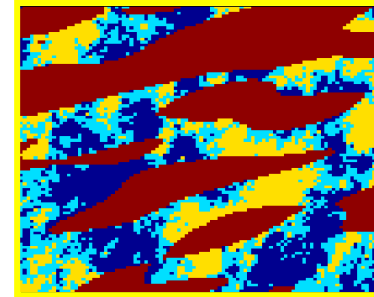
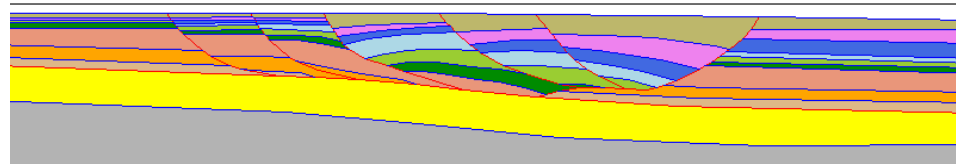
Conservation de la masse

Conservation du volume de pore

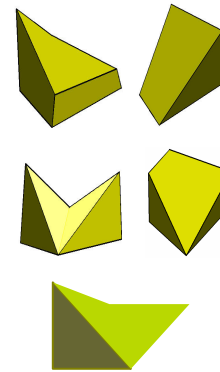
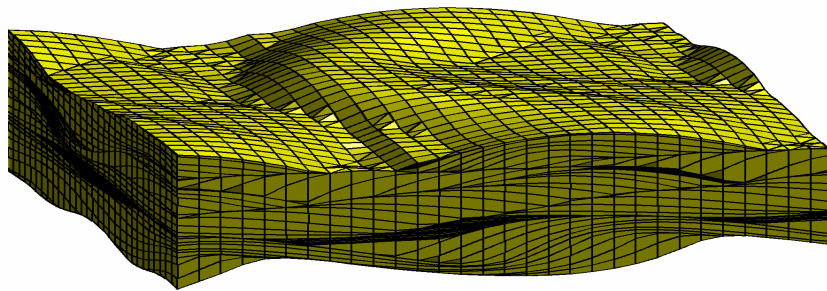
+ Equilibre thermodynamique

Géométries-Maillages

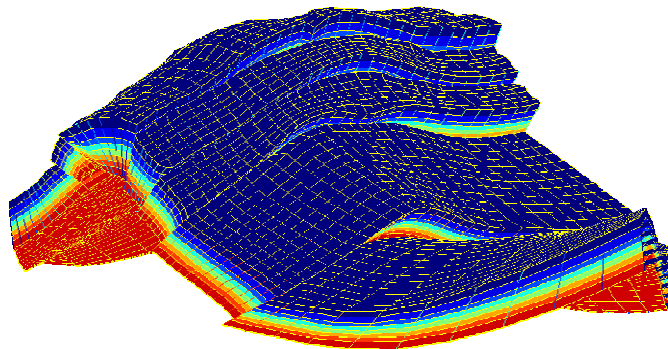
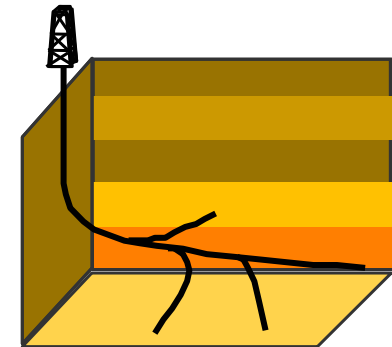
Milieux stratifiés hétérogènes
anisotropes



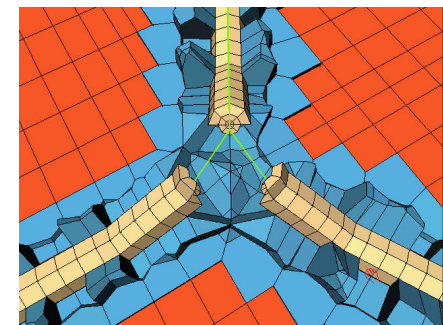
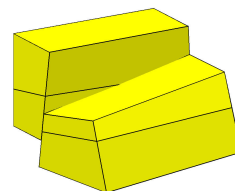
Erosions



Puits



Failles

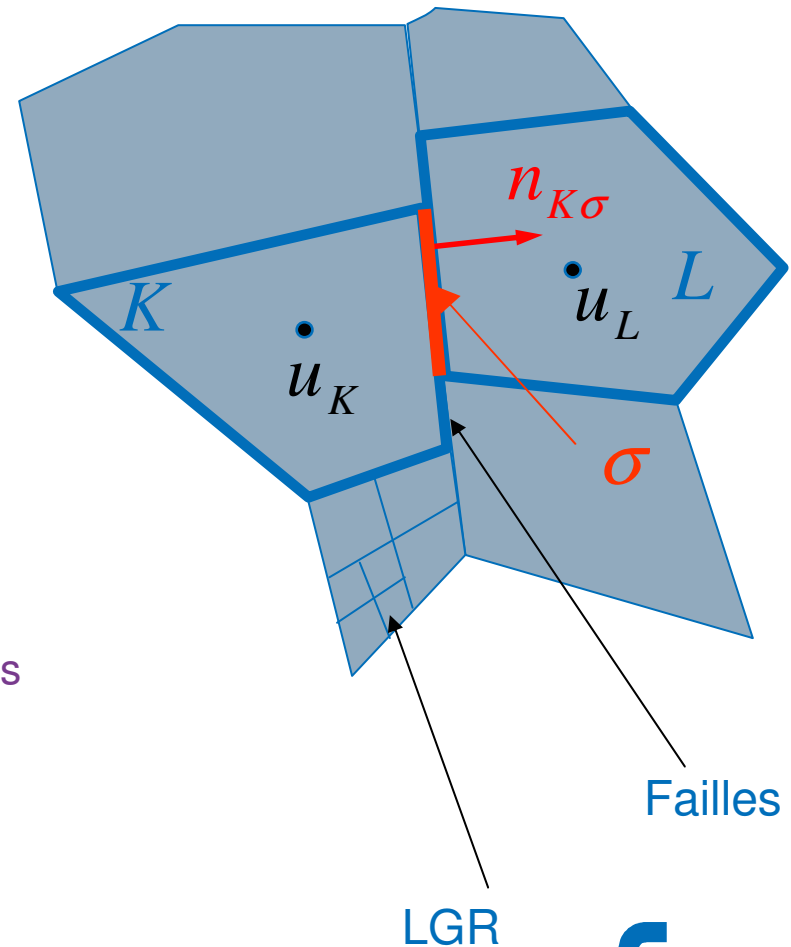


Discrétisation volume fini des flux diffusifs

$$\int_{\sigma} -K \nabla u \cdot n_{K,\sigma} ds = \sum_{M \in T_{\sigma}} T_{K,\sigma}^M u_M$$

$$u = P, P_{c,\alpha}(S), C_i^{\alpha}, T$$

- Maillages généraux
- Milieu hétérogène, anisotrope
- Coût et robustesse
 - Stencil compact, schémas centrés
 - Coercivité
 - Monotonicité



Systemes non lineaires et lineaires

$$X = (X_K)_{K \in T} = (P_K, S_K^\alpha, C_K^\alpha)_{K \in T}$$

$$\begin{cases} M_K (X_K^{n+1}) + \sum_{\sigma \in \Sigma_K} F_{K,\sigma} (P^{n+1}, S^*, C^*) = 0 \\ C_K (X_K^{n+1}) = 0 \end{cases} \quad * = n, n + 1$$

- **Systeme non lineaire** 5 à 50% du temps calcul
 - Algorithme de type Newton
 - Gestion des changements de phase par le Flash thermodynamique
- **Systeme lineaire** ← 80 à 50% du temps calcul
 - Réduction du systeme par élimination des lois de fermeture et des inconnues explicites

Méthode Combinative-AMG

$$\begin{pmatrix} J_{pp} & J_{pc} \\ J_{cp} & J_{cc} \end{pmatrix} \begin{pmatrix} Y_p \\ Y_c \end{pmatrix} = \begin{pmatrix} b_p \\ b_c \end{pmatrix}$$

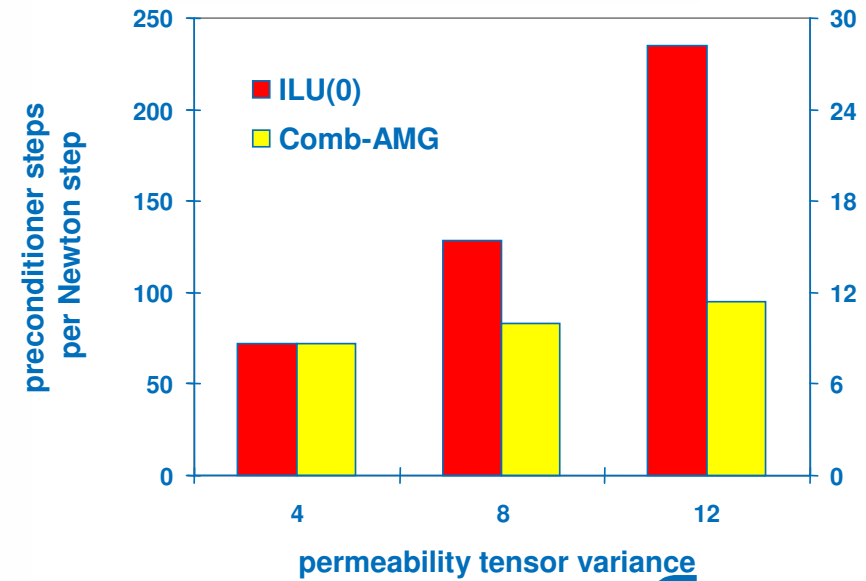
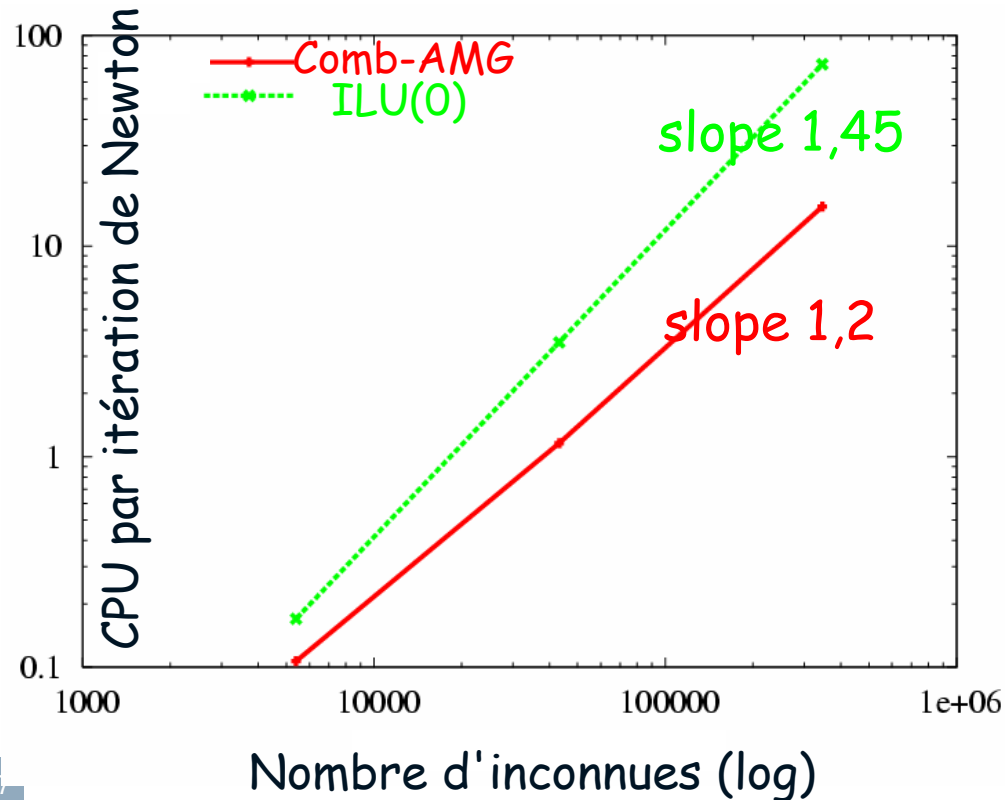
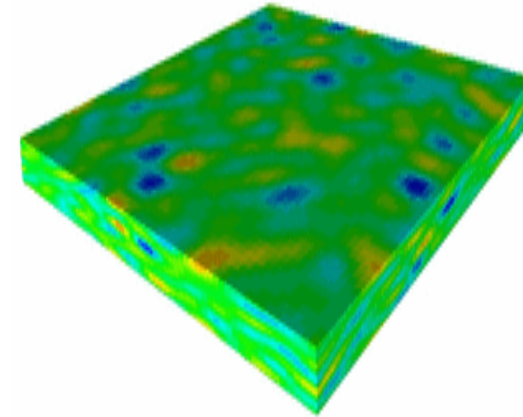
$$\begin{pmatrix} Y_p^{(1)} \\ Y_c^{(1)} \end{pmatrix} = C_{ILU(0)}^{-1} \begin{pmatrix} b_p \\ b_c \end{pmatrix} \quad \text{Préconditionnement ILU(0) du système}$$

$$Y_p^{(2)} = C_{AMG}^{-1} \left(b_p - J_{pp} Y_p^{(1)} - J_{cp} Y_c^{(1)} \right) \quad \text{Vcycle(s) AMG sur le bloc pression}$$

$$\begin{pmatrix} Y_p \\ Y_c \end{pmatrix} = \begin{pmatrix} Y_p^{(1)} + Y_p^{(2)} \\ Y_c^{(1)} \end{pmatrix} = \left[C_{ILU(0)}^{-1} + \begin{pmatrix} C_{AMG}^{-1} & 0 \\ 0 & 0 \end{pmatrix} (I - J C_{ILU(0)}^{-1}) \right] b$$

Cas test synthétiques Black Oil en simulation de réservoir

- Modèle Black Oil (3 inconnues par maille)
- Champ de perméabilité log-normal
- Maillage Cartésien





Couplage écoulement transport réactif

$$X_e = X_f \quad \text{Système RS: réactions hétérogènes w-g de type changement de phase}$$

$$\sum_{e \in \mathcal{E}_w} A_{r,e} X_e + \sum_{m \in \mathcal{M}} A_{r,m} X_m = 0, \quad r \in \mathcal{R}^{TR} \quad \text{Système TR: réactions en phase aqueuse et interactions eau roche}$$

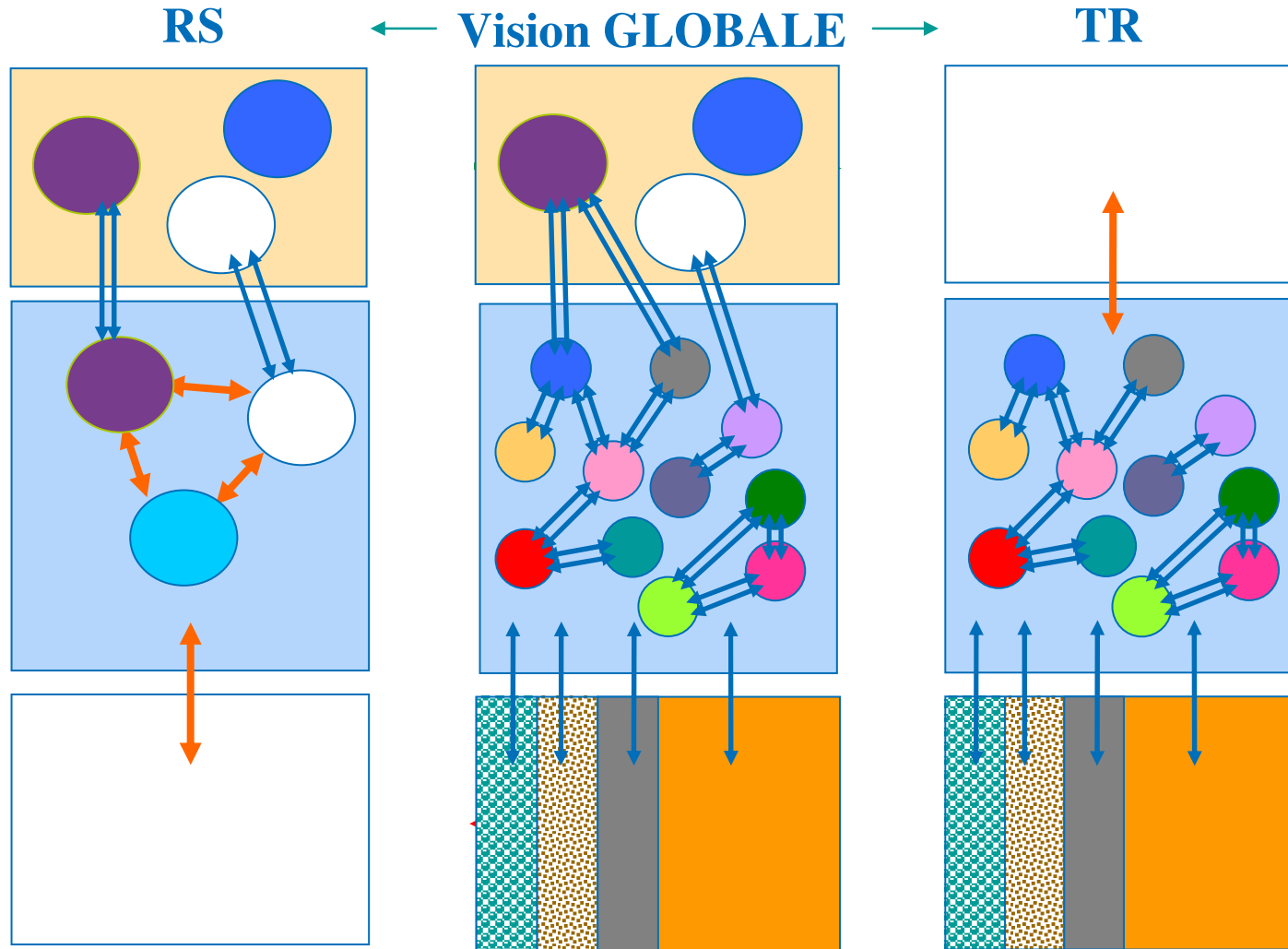
$$\partial_t (\phi \rho_g S_g C_e) + \text{div}(\rho_g C_e \mathbf{V}_g) + \text{div}(-\phi \rho_g S_g \mathcal{D}_e \nabla C_e) + T_e^{RS} = 0 \quad \text{espèces gazeuses } e$$

$$\partial_t (\phi \rho_w S_w C_e) + \text{div}(\rho_w C_e \mathbf{V}_w) + \text{div}(-\phi \rho_w S_w \mathcal{D}_e \nabla C_e) \quad \text{espèces aqueuses } e$$

$$+ T_e^{RS} + T_e^{TR} + Q_e^{TR} = 0$$

$$\partial_t (\phi_m \rho_m) + T_m^{TR} + Q_m^{TR} = 0 \quad \text{minéraux } m$$

Stratégie de résolution découplée du système réactif



SLEIPNER

MINERAL COMPOSITION OF THE SAND

Nordland shale composition (after Pearce and others, 1999)	Volume fraction	Minerals introduced in the model	Volume in the fraction
Plagioclase	0.0301	Albite~low	0.030
Calcite	0.0674	Calcite	0.067
Quartz	0.7633	Chalcedony	0.769
Chlorite	0.0133	Chlorite	0.013
Mica/Illite	0.0522	Muscovite	0.052
K-feldspar	0.0693	K-feldspar	0.069
Pyrite	0.0005	Not used	--
Ilmenite	0.0012	Not used	--
Apatite	0.0002	Not used	--
Zeolite	0.0022	Not used	--
Ti Oxides	0.0003	Not used	--
Siderite	--	Siderite	0.000
Kaolinite	--	Kaolinite	0.000
Dolomite-dis	--	Dolomite-dis	0.000
Magnesite	--	Magnesite	0.000
Dawsonite	--	Dawsonite	0.000

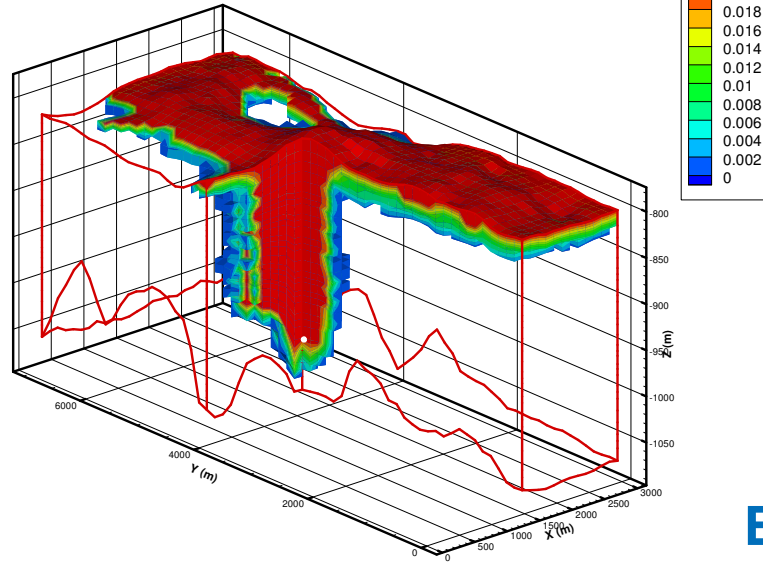
SLEIPNER MINERAL COMPOSITION OF THE SHALE

Nordland shale composition (after Bøe and Zweigel, 2001)	Volume percent	Minerals introduced in the model	Volume percent
Plagioclase	0.132	Albite~low	0.132
Calcite	0.010	Calcite	0.010
Quartz	0.228	Chalcedony	0.334
Chlorite	0.044	Chlorite	0.044
Mica/Illite	0.251	Muscovite	0.251
Kaolinite	0.195	Kaolinite	0.195
K-feldspar	0.023	K-feldspar	0.023
Siderite	0.011	Siderite	0.011
Smectite	0.09	Not used	--
Pyrite	0.016	Not used	--
Dolomite-dis	--	Dolomite-dis	0.000
Magnesite	--	Magnesite	0.000
Dawsonite	--	Dawsonite	0.000



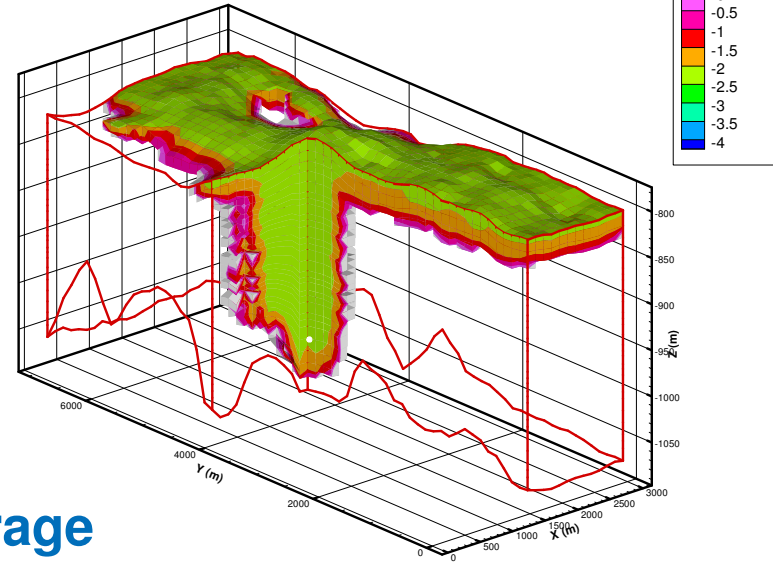
W-CO2

End of CO2 injection



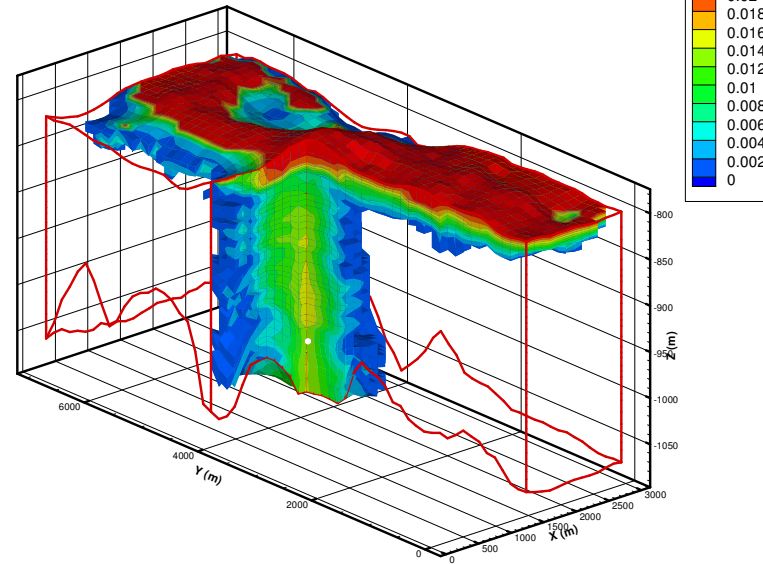
End of injection

End of CO2 injection

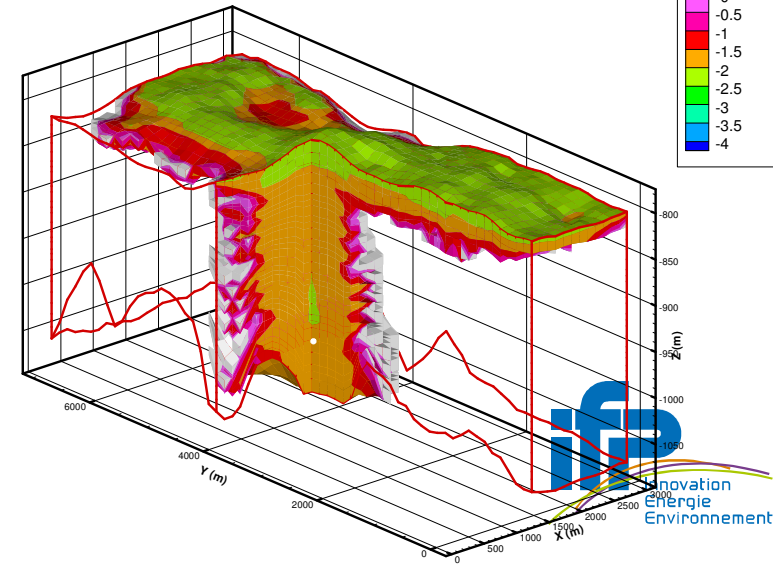


End of storage

End of CO2 storage



End of CO2 storage



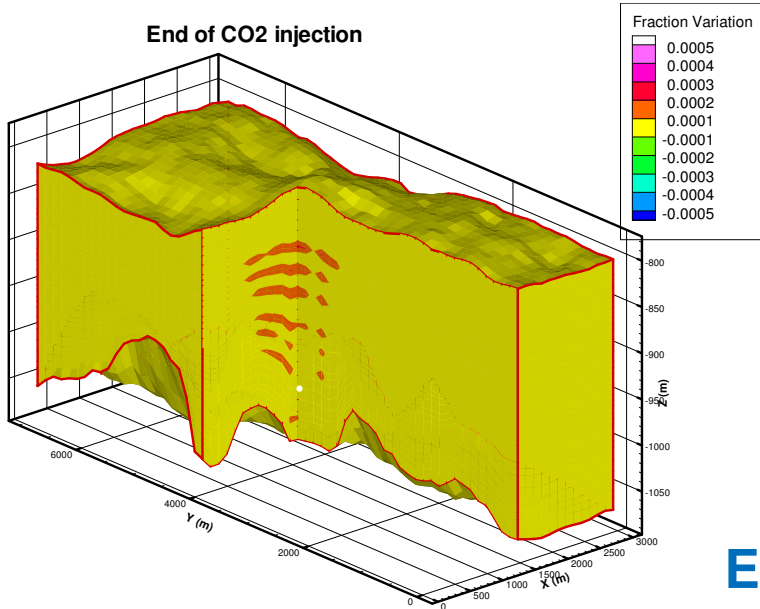


Kaolinite

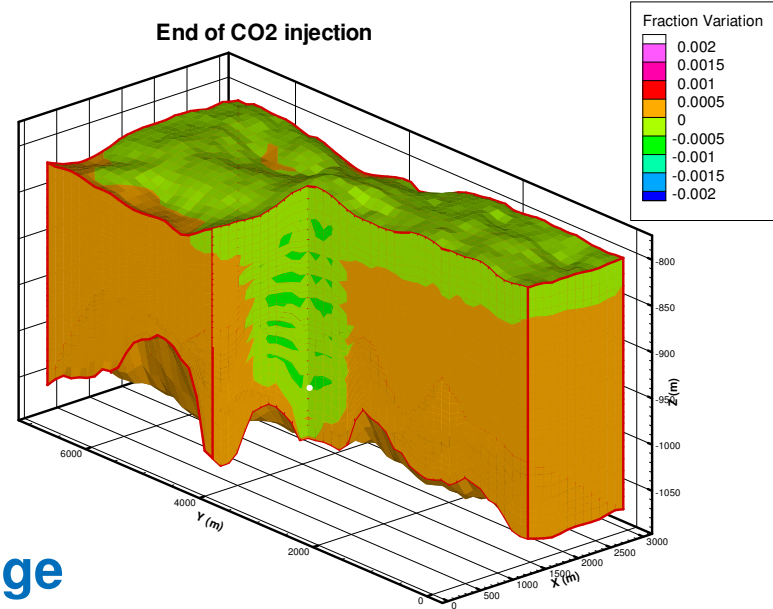
End of injection

Calcite

End of CO2 injection

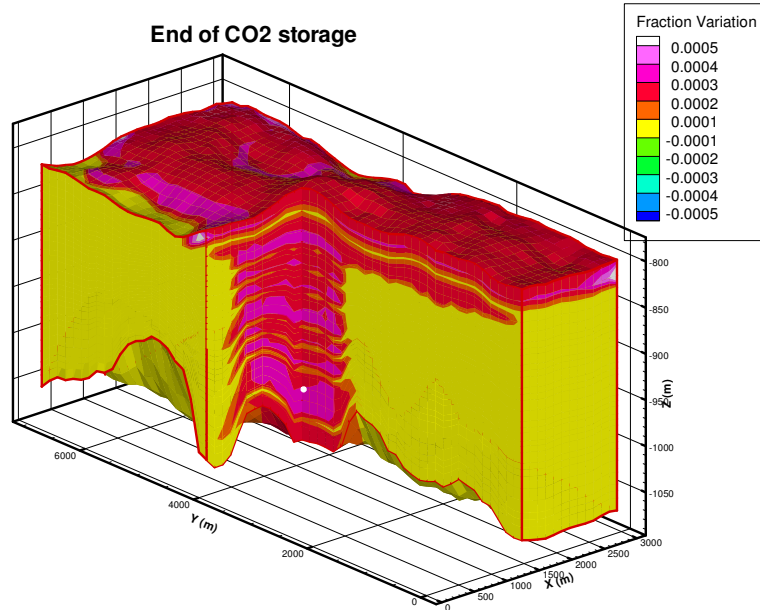


End of CO2 injection

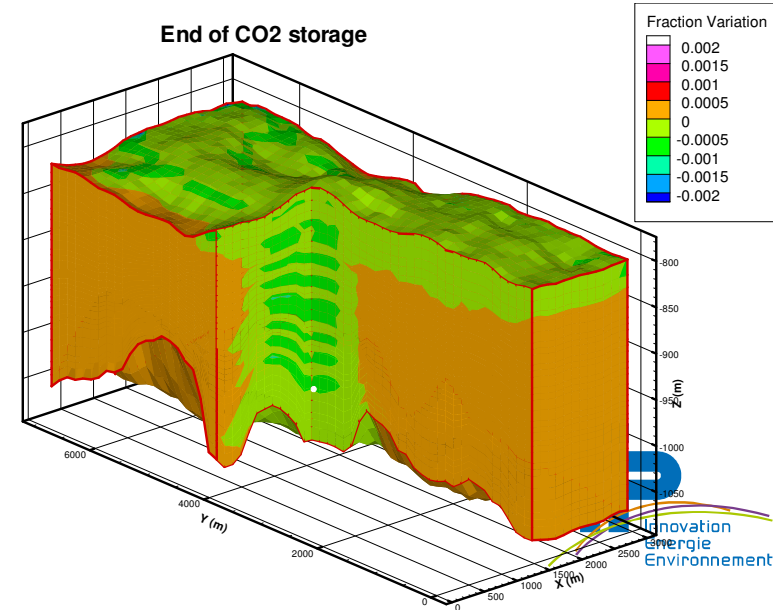


End of storage

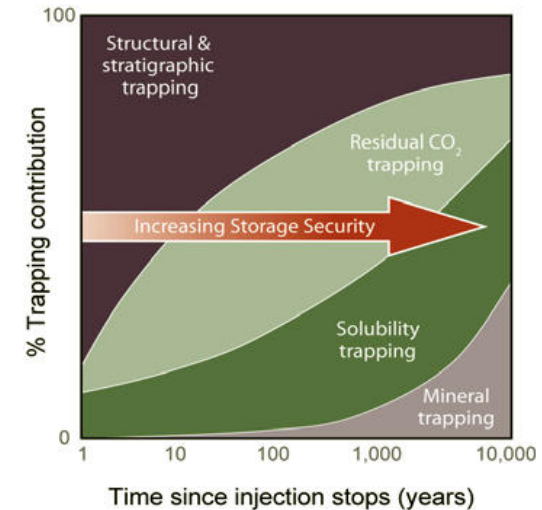
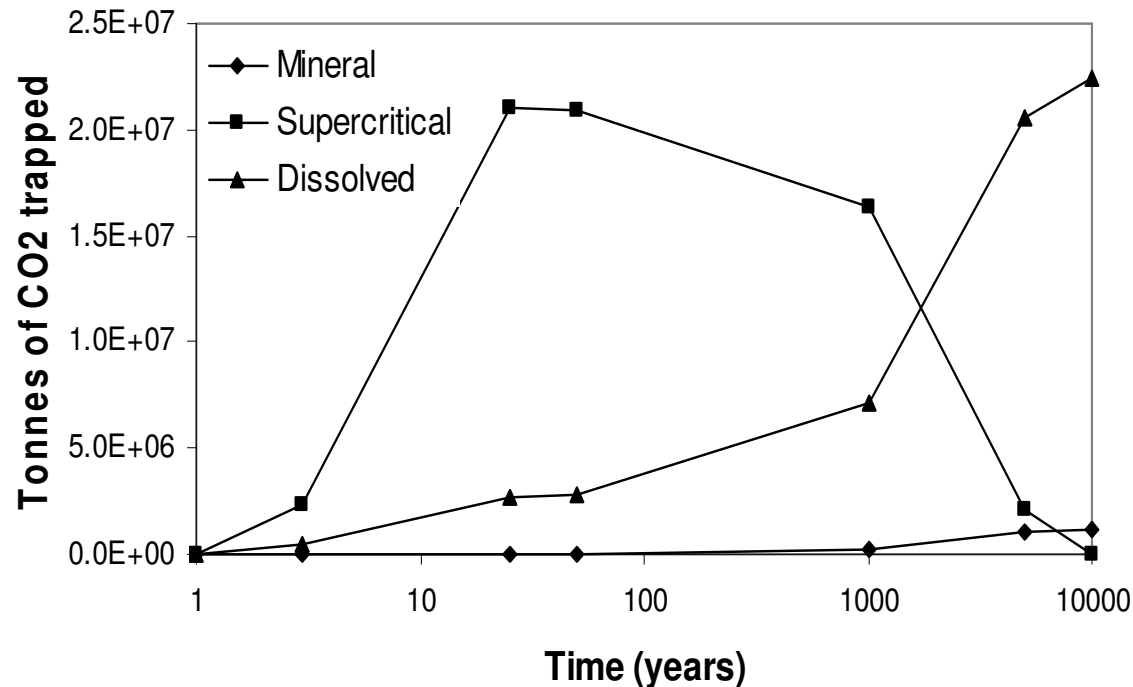
End of CO2 storage



End of CO2 storage



Sleipner: amount of CO₂ stored (Pascal Audigane BRGM)



Total amounts of carbon dioxide present as a free (supercritical) gas phase, dissolved in the aqueous phase, and trapped in carbonated minerals (dawsonite mainly).

Dissolution trapping plays a major role in the long term, while mineral trapping is minor at Sleipner.

Conclusions



- Modèles avec de nombreux couplages
 - Hydrodynamique
 - Thermodynamique
 - Géochimie
 - Géomécanique

- Echelles spatiales et temporelles hétérogènes
 - Milieu hétérogène anisotrope
 - Puits, bassin, failles, couverture
 - Injection, stockage
 - Physiques

- Prédications difficiles à moyen et long terme
 - Peu de données sur la géologie (hétérogénéités, géométrie des barrières, ...) la géochimie, la pétrophysique, ...
 - Importance du Monitoring



Conclusions

Bilan des difficultés pour la simulation

- Front de migration – dissolution de la bulle de gaz
- Apparition et disparition de phases (Darcy, Diffusion)
- Instabilités gravitaires
- Convection diffusion-dispersion des espèces aqueuses
- Discrétisation sur maillages proches puits
- Couplage écoulement diphasique transport réactif
- Formulation et résolution du transport réactif
- Couplage avec la géomécanique
- Milieu hétérogène anisotrope, échelles du puits et du bassin