

# Simulations des cas tests diphasiques MoMaS

## Résultats et discussions

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## Modélisation des écoulements liquide-gaz en milieu poreux

Hypothèses physiques

Choix des variables principales

### Résolution

Formulation mathématique

Implémentation

### Résultats des cas tests

Cas test I.a

Cas test I.b

Cas test II.b

Cas test III.a

Cas test III.b

### Propositions de cas tests

Pressions d'entrées

Effet du jeu

Modélisation

Résolution

Cas tests

Propositions

## Hypothèses générales

- ▶ 2 phases : liquide et gaz
- ▶  $N+1$  composants : 1 solvant (*liquide*) et  $N$  solutés (*gaz*)
- ▶ Equilibre thermodynamique local entre la solution liquide et le mélange gazeux
- ▶ Loi de pression capillaire "*univoque*" :  $P_g - P_l = P_c(S_g)$
- ▶ Conservation de la masse pour chaque composant
- ▶ Transport par convection et diffusion de chaque composant dans chaque phase
- ▶ Loi de Darcy généralisée pour l'écoulement de chaque phase
- ▶ Pas de réactions chimiques

### Hypothèses simplificatrices actuelles

- ▶ Matrice poreuse indéformable
- ▶ Mélange idéal de gaz parfaits pour la phase gaz
- ▶ Solution idéale pour la phase liquide (composants gazeux peu solubles)
- ▶ Phase liquide incompressible
- ▶ Ecoulement isotherme

### ► Bilan des inconnues/reliations

- Description d'une phase en milieu poreux :

$$S_\alpha, P_\alpha, c_\alpha, (x_\alpha^i)_{i=1..N}$$

- 3+N inconnues par phase

- Equation d'état pour chaque phase :  $c_\alpha = \left( \sum_i v_\alpha^i x_\alpha^i \right)^{-1}$

- 1 relation par phase

- Les phases saturent les pores :  $S_g + S_l = 1$

- 1 relation

- Loi de pression capillaire :  $P_g - P_l = P_c(S_g)$

- 1 relation

- Equilibre entre phases :  $x_g^i P_g = K^i x_l^i$

- N+1 relations

- Conservation de la masse pour chaque composant

- N+1 relations

### ► "Localement" : N+1 degrés de liberté

# Modélisation

## Choix des variables principales

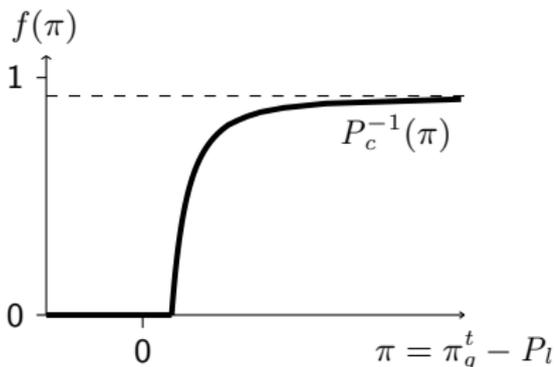
Détermination de l'état saturé/insaturé avec le jeu de variables

$$(P_l, (x_l^i)_{i=1..N})$$

► Si gaz et liquide coexistent :

- Equilibre thermodynamique ( $x_g^i P_g = K^i x_l^i$ ) :  $\pi_g^t = \sum_i K^i x_l^i$
- Equilibre "mécanique" :  $\pi_g^m = P_l + P_c(S_g)$

► Compatibilité des équilibres si  $P_l + P_c^{min} \leq \pi_g^t \leq P_l + P_c^{max}$



$$S_g \equiv f(\pi_g^t - P_l)$$

Intérêt du jeu de variables  $(P_l, (x_l^i)_{i=1..N})$

- ▶ Variables physiques tant que la phase liquide est présente ( $S_l > 0$ )
- ▶ Pas de discontinuité *a priori* aux interfaces de roches

Le problème peut s'écrire sous la forme d'un système d'edp "quasi linéaire"

$$\frac{\partial b_i(\mathbf{u})}{\partial t} - \operatorname{div} \left( \sum_j A_{i,j}(\mathbf{u}) \nabla u_j - u_i \sum_j C_{i,j}(\mathbf{u}) \nabla u_j \right) = F_i, \quad i = 0..N$$

Pour un schéma implicite en temps,  $\mathbf{u}^n \approx \mathbf{u}(t^n)$  peut être approché par un point fixe de la forme (itérer sur  $k$ )

$$\begin{aligned} & - \operatorname{div} \left( \sum_j A_{i,j}(\mathbf{u}^{n,k-1}) \nabla u_j^{n,k} - u_i^{n,k} \sum_j C_{i,j}(\mathbf{u}^{n,k-1}) \nabla u_j^{n,k-1} \right) \\ & + \Delta t^{-1} \sum_j J_{i,j}(u_i^{n,k-1}) u_i^{n,k} = Q_i(\Delta t, \mathbf{u}^{n-1}, \mathbf{u}^{n,k-1}), \quad i = 0..N \end{aligned}$$

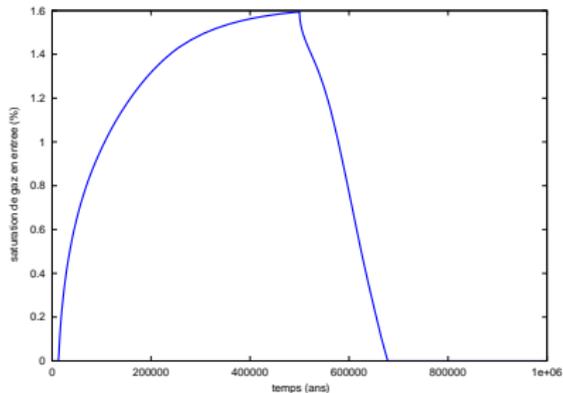
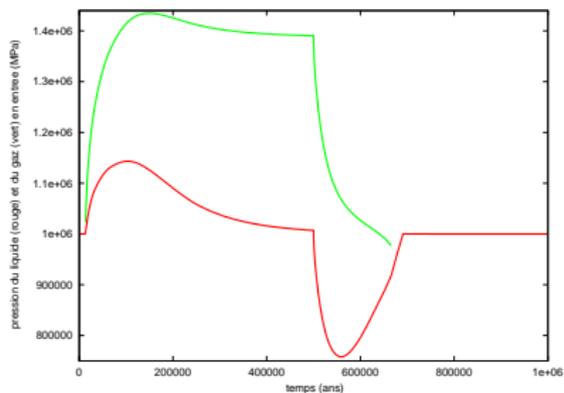
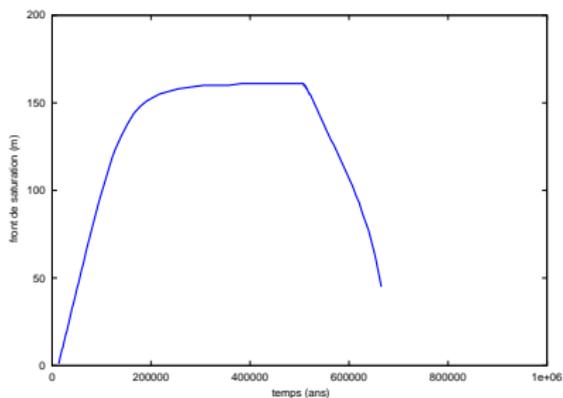
Il "suffit" de résoudre cette edp linéaire avec le schéma de son choix...

- ▶ Développement d'une bibliothèque C++
  - ▶ Découplage des différents aspects
    - "modèles physiques"
    - "formulation mathématique"
    - "discrétisation spatiale"
  - ▶ Utilisation de la bibliothèque C++ *LibMesh*
    - ▶ Gestion des maillages, matrices, solveurs linéaires
    - ▶ Schémas éléments finis, raffinement de maillage
    - ▶ Exécutable indépendant de la dimension
- ▶ Actuellement :
  - ▶ Formulation en pression liquide / fraction molaire des gaz dissouts :  $(P_l, (x_l^i)_{i=1..N})$
  - ▶ Schéma éléments finis Lagrange

# Résultats des cas tests

## Cas test I.a

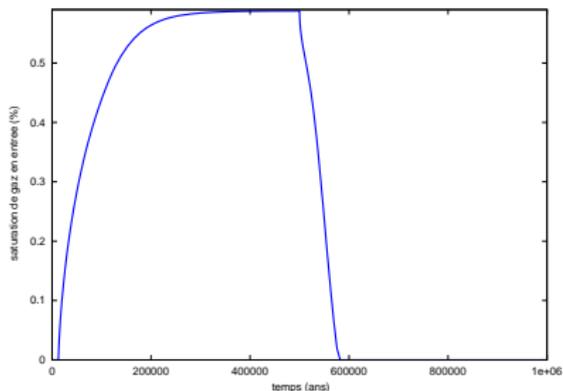
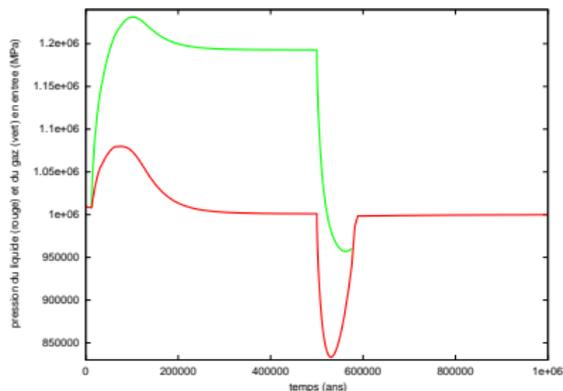
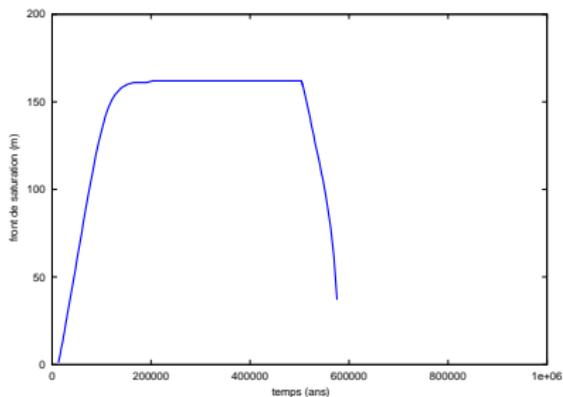
$$\begin{array}{l} \phi^w \cdot \mathbf{n} = 0 \\ \phi^h \cdot \mathbf{n} = \phi_{in}^h \end{array} \quad \boxed{P_l = P_{l,out} ; x_l^h = 0} \quad \begin{array}{l} P_l = P_{l,out} \\ x_l^h = 0 \end{array}$$



# Résultats des cas tests

## Cas test I.a + vapeur d'eau

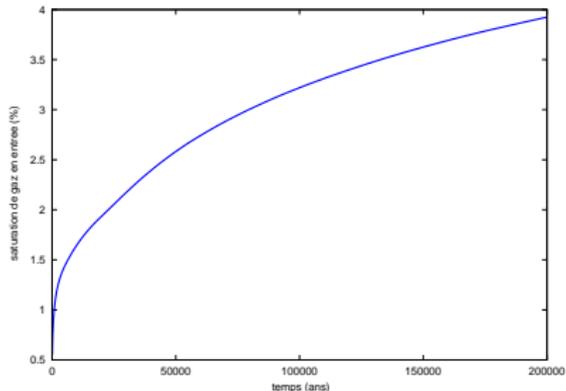
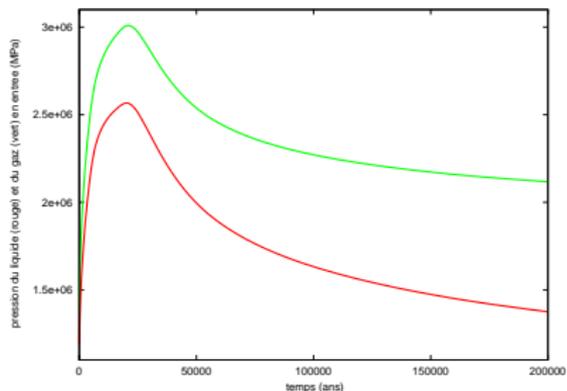
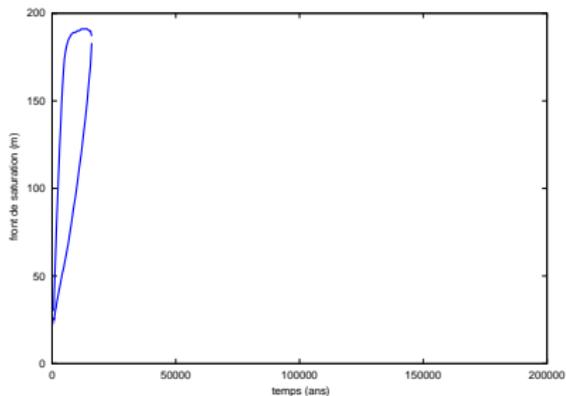
$$\begin{array}{l} \phi^w \cdot \mathbf{n} = 0 \\ \phi^h \cdot \mathbf{n} = \phi_{in}^h \end{array} \quad \boxed{P_l = P_{l,out} ; x_l^h = 0} \quad \begin{array}{l} P_l = P_{l,out} \\ x_l^h = 0 \end{array}$$



# Résultats des cas tests

## Cas test I.b

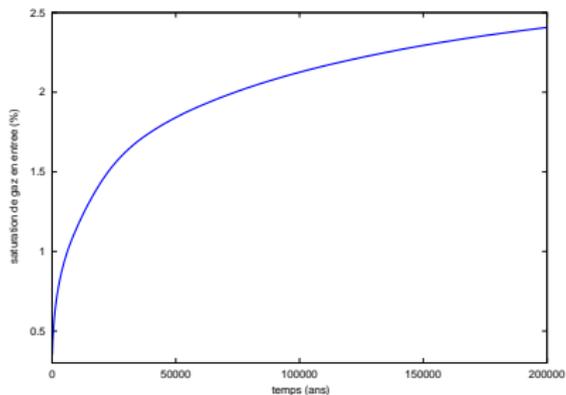
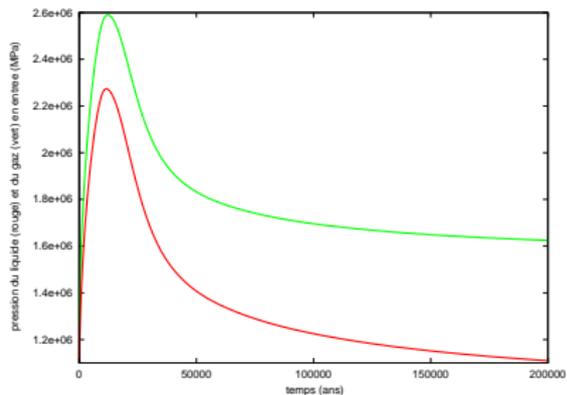
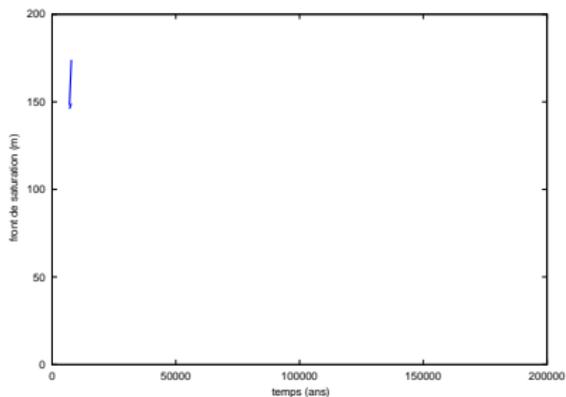
$$\begin{array}{l} \phi^w \cdot \mathbf{n} = 0 \\ \phi^h \cdot \mathbf{n} = \phi_{in}^h \end{array} \left[ \begin{array}{l} P_l = P_{l,out} ; P_g = P_{g,out} \\ P_l = P_{l,out} \\ P_g = P_{g,out} \end{array} \right.$$



# Résultats des cas tests

## Cas test I.b + vapeur d'eau

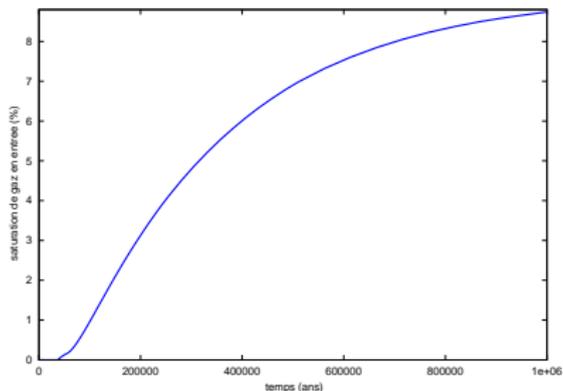
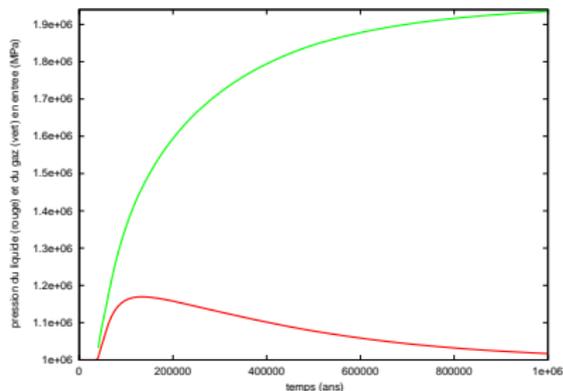
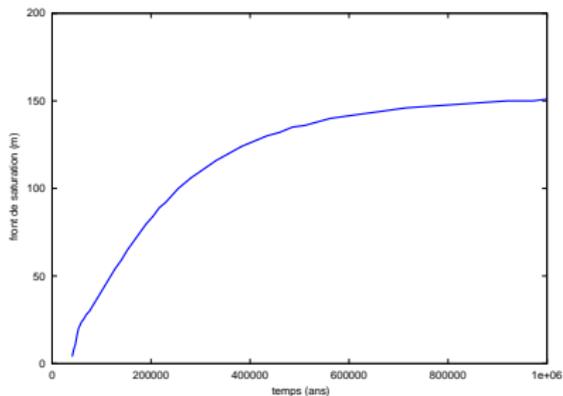
$$\begin{array}{l} \phi^w \cdot \mathbf{n} = 0 \\ \phi^h \cdot \mathbf{n} = \phi_{in}^h \end{array} \left\{ \begin{array}{l} P_l = P_{l,out} ; P_g = P_{g,out} \\ P_l = P_{l,out} \\ P_g = P_{g,out} \end{array} \right.$$



# Résultats des cas tests

## Cas test II.b

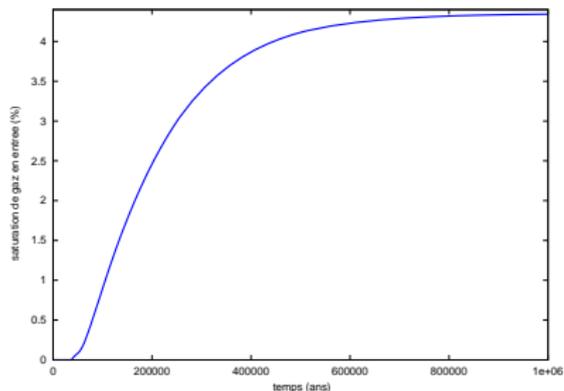
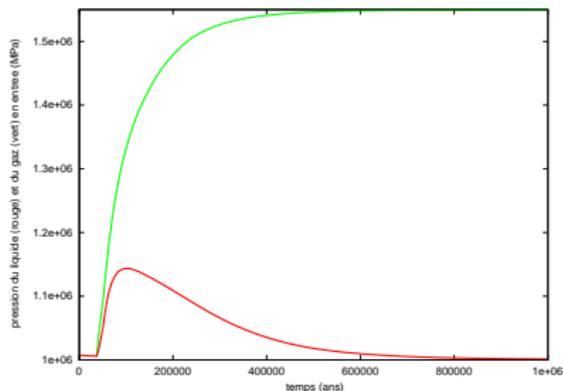
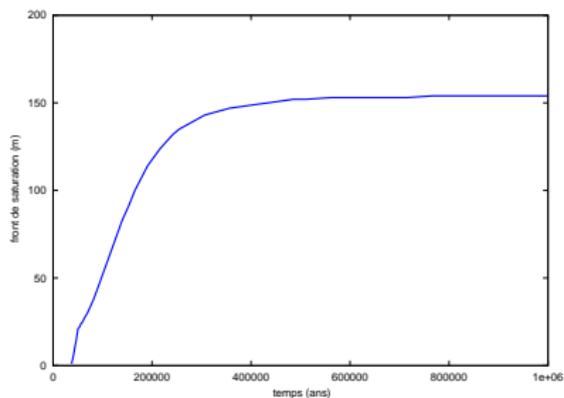
$$\begin{array}{l} \phi^w \cdot \mathbf{n} = 0 \\ \phi^h \cdot \mathbf{n} = \phi_{in}^h \end{array} \left[ \begin{array}{c|c} \Omega_b & \Omega_c \\ \hline P_l = P_{l,out} ; x_l^h = 0 & P_l = P_{l,out} \\ x_l^h = 0 & x_l^h = 0 \end{array} \right]$$



# Résultats des cas tests

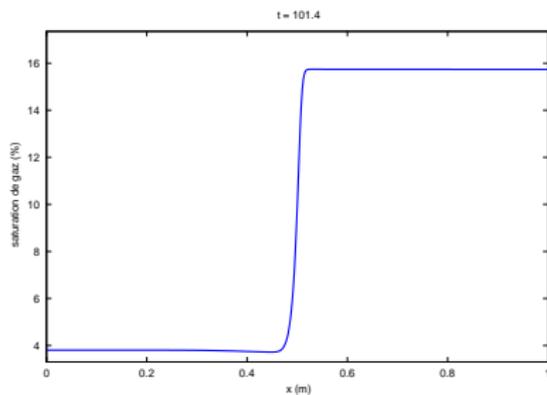
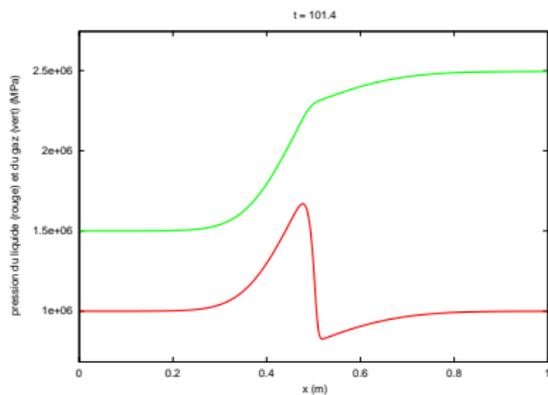
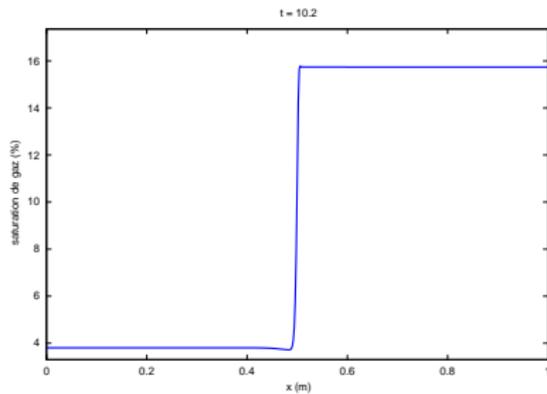
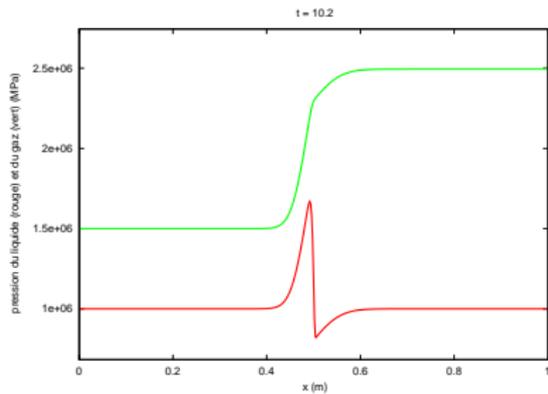
## Cas test II.b + vapeur d'eau

$$\begin{array}{l} \phi^w \cdot \mathbf{n} = 0 \\ \phi^h \cdot \mathbf{n} = \phi_{in}^h \end{array} \quad \boxed{\begin{array}{c} \Omega_b \quad | \quad \Omega_c \\ P_l = P_{l,out} ; \quad x_l^h = 0 \end{array}} \quad \begin{array}{l} P_l = P_{l,out} \\ x_l^h = 0 \end{array}$$



# Résultats des cas tests

## Cas test III.a



# Résultats des cas tests

## Cas test III.a

Simulations des cas tests diphasiques MoMaS

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Modélisation

Résolution

Cas tests

I.a

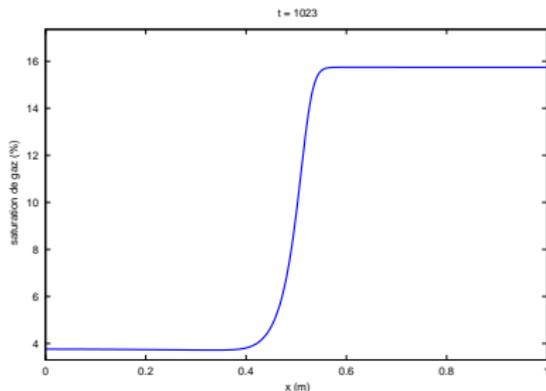
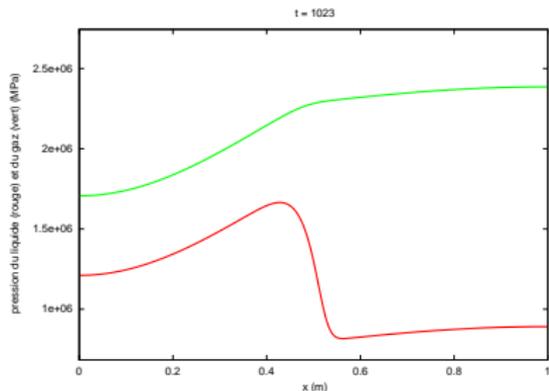
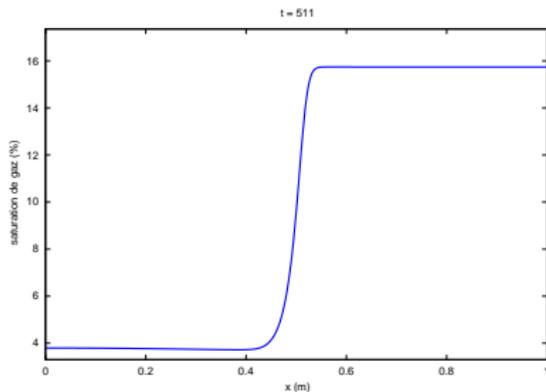
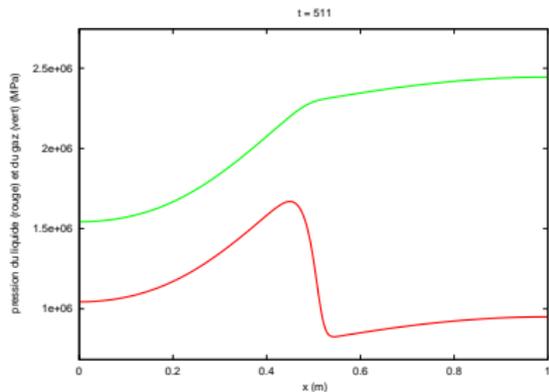
I.b

II.b

III.a

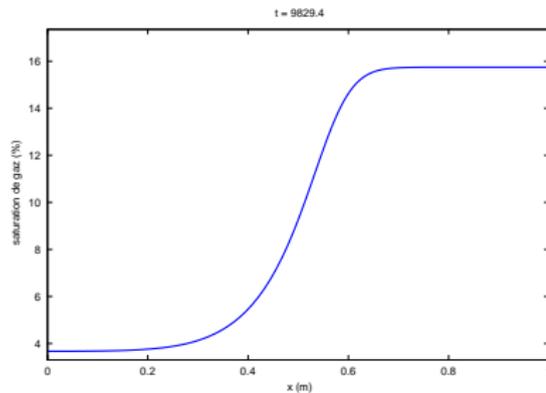
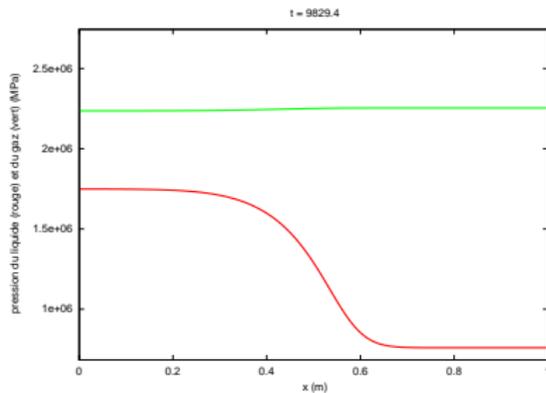
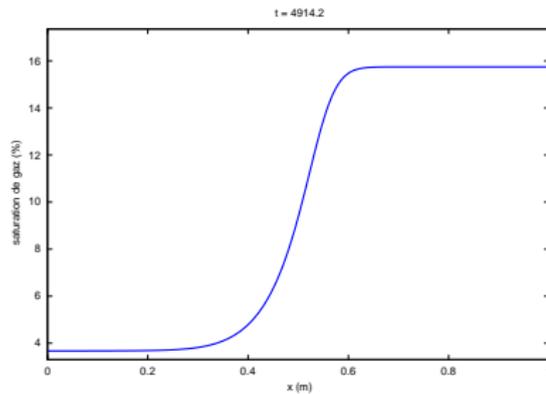
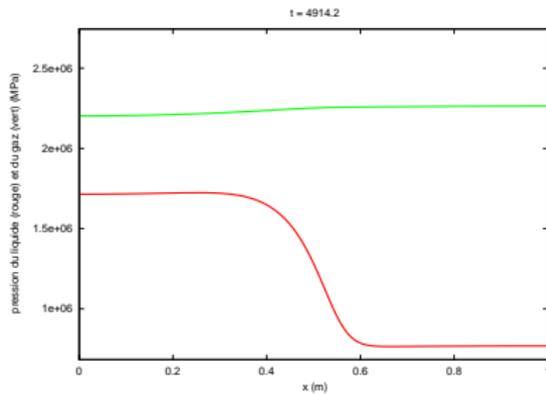
III.b

Propositions



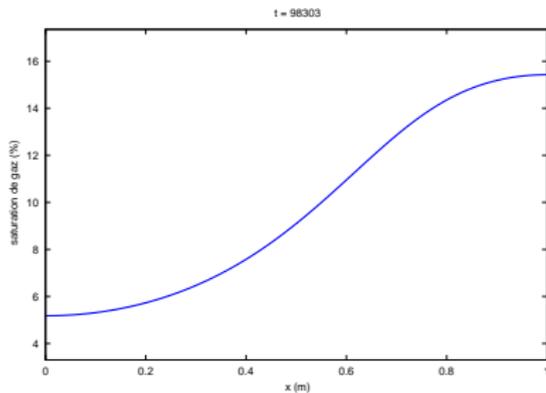
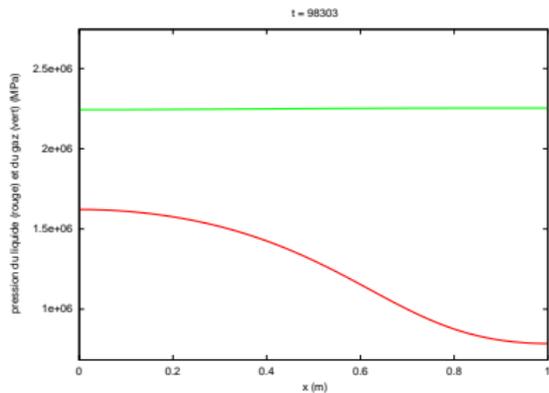
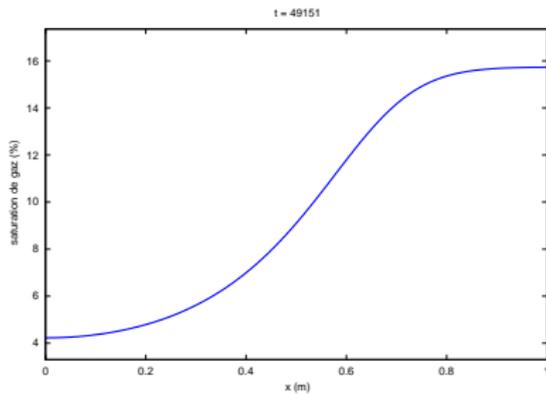
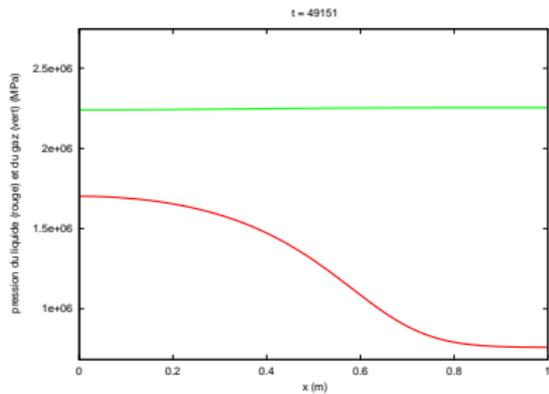
# Résultats des cas tests

## Cas test III.a



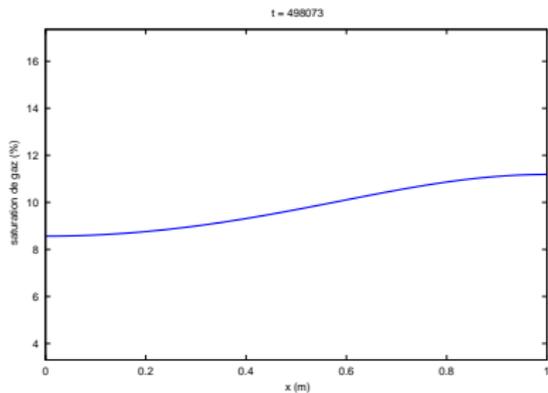
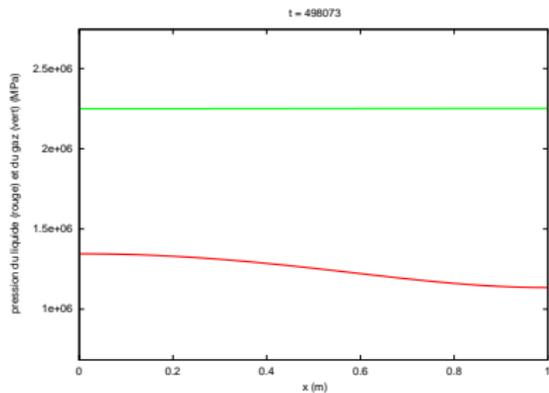
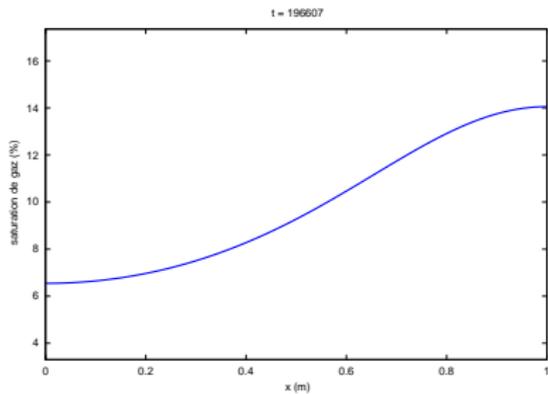
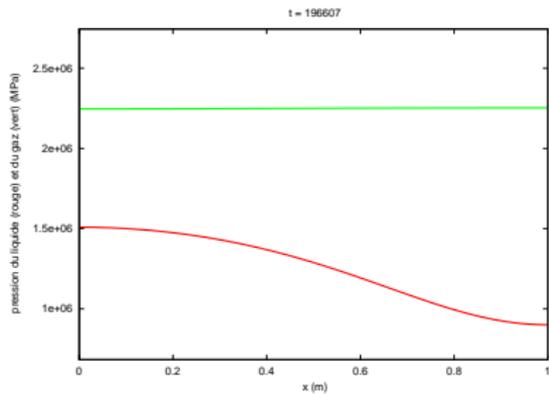
# Résultats des cas tests

## Cas test III.a



# Résultats des cas tests

## Cas test III.a



# Résultats des cas tests

## Cas test III.a

Simulations des cas tests diphasiques  
MoMaS

Alain Bourgeat,  
Magdalena  
Dymitrowska, **Farid  
Smaï**

Modélisation

Résolution

Cas tests

I.a

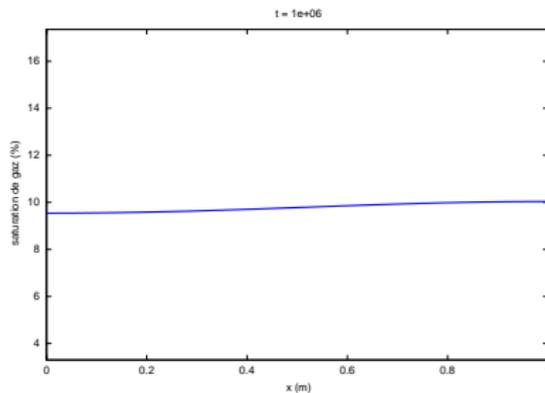
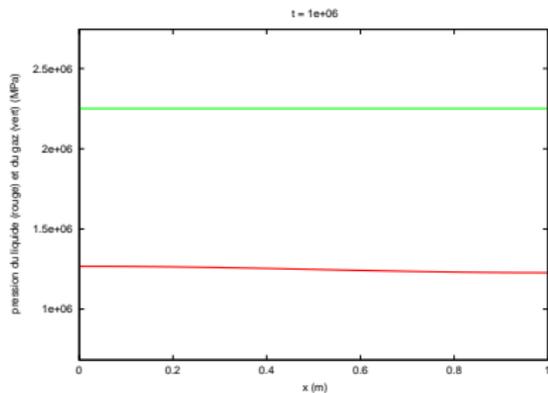
I.b

II.b

III.a

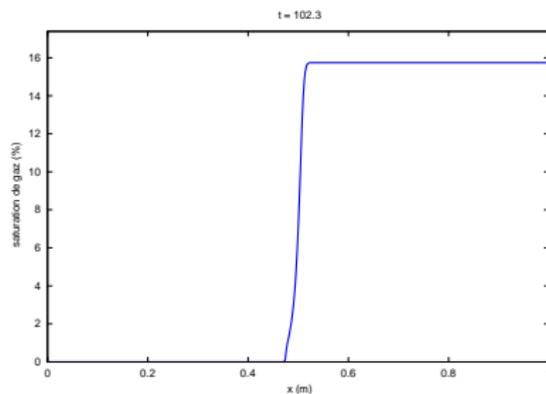
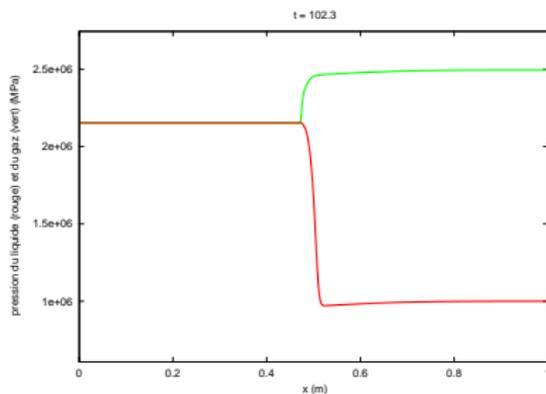
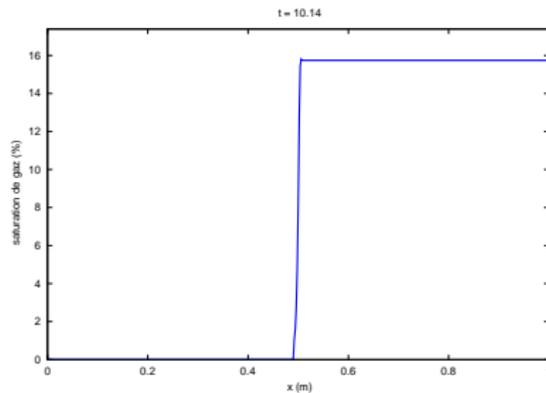
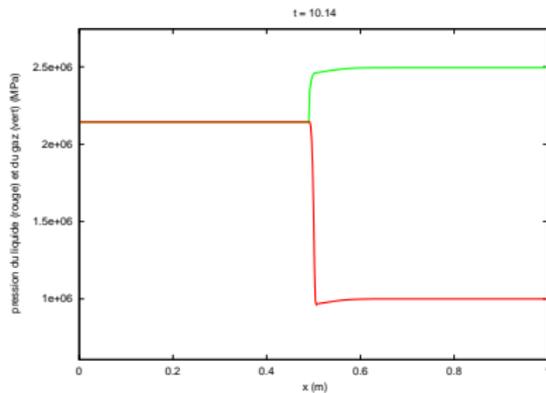
III.b

Propositions



# Résultats des cas tests

## Cas test III.b



# Résultats des cas tests

## Cas test III.b

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Cas tests

I.a

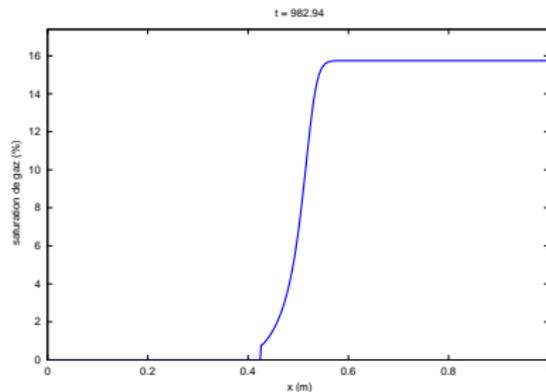
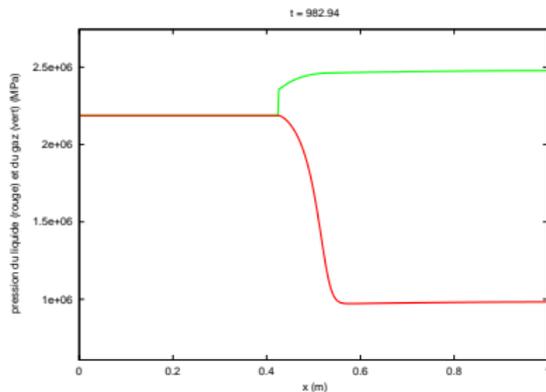
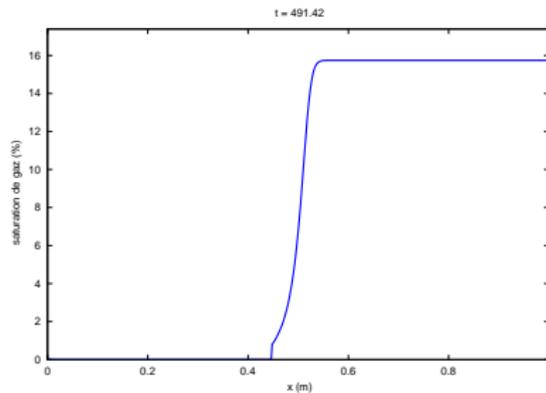
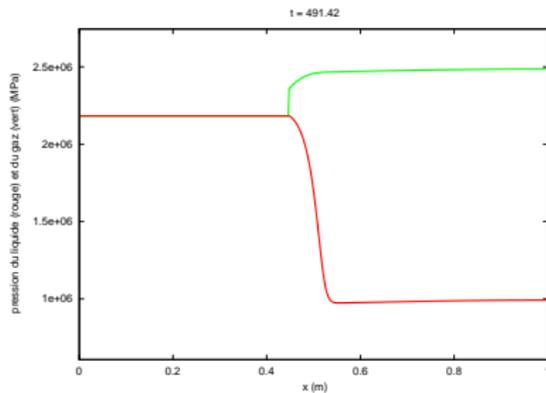
I.b

II.b

III.a

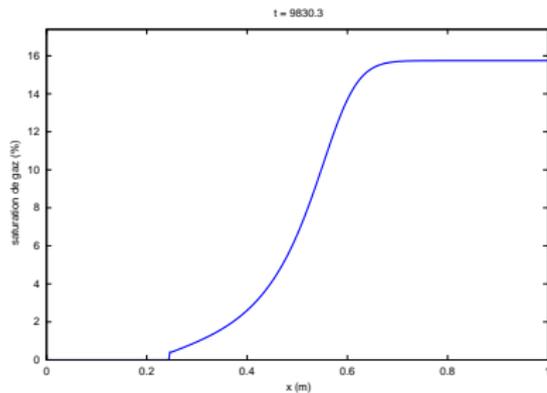
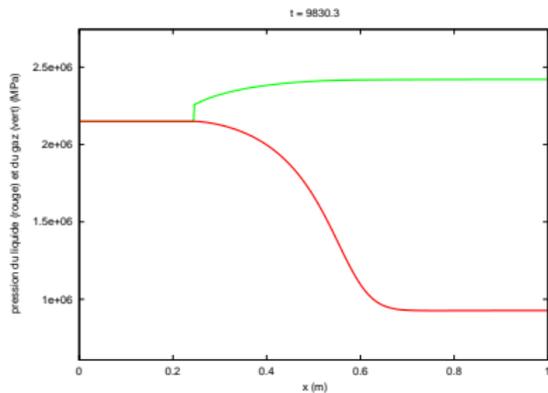
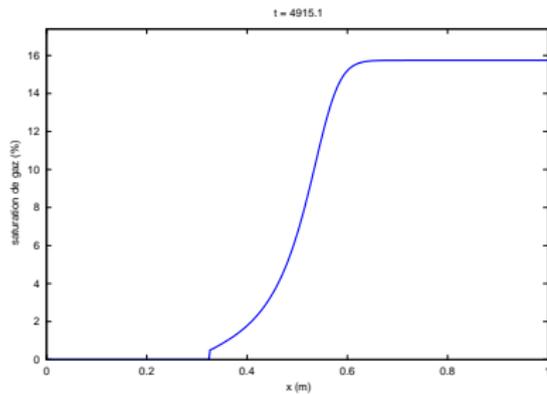
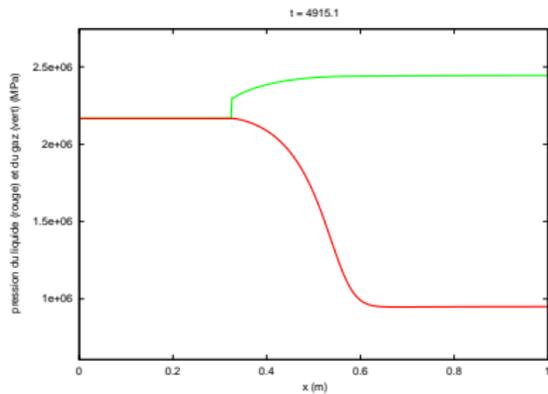
III.b

Propositions



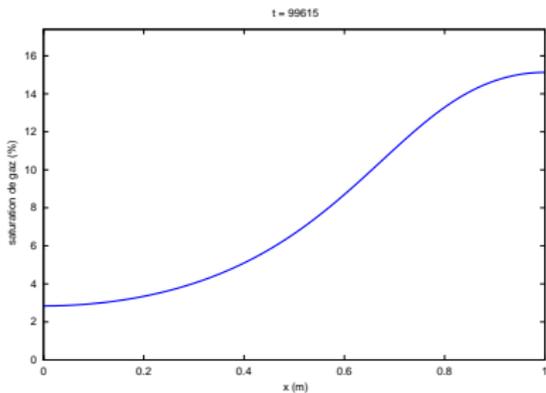
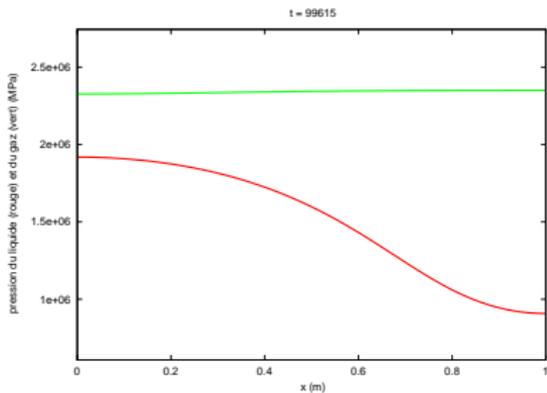
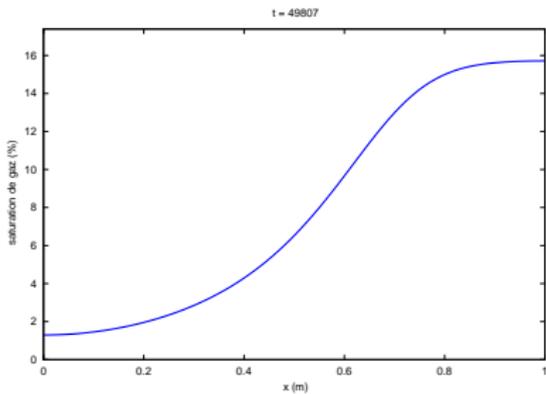
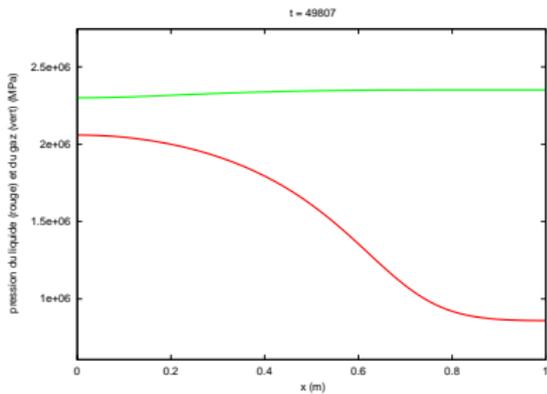
# Résultats des cas tests

## Cas test III.b



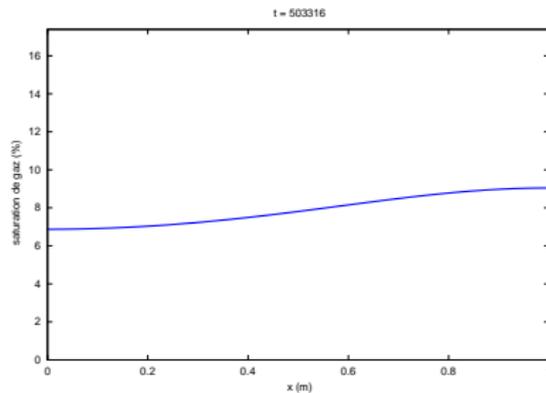
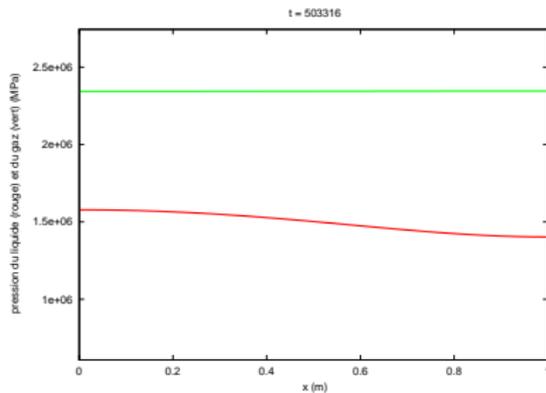
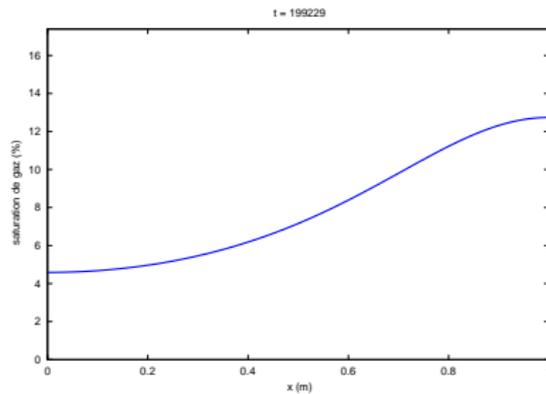
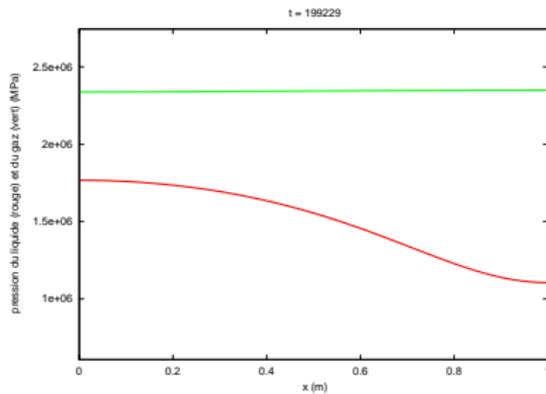
# Résultats des cas tests

## Cas test III.b



# Résultats des cas tests

## Cas test III.b



# Résultats des cas tests

## Cas test III.b

Modélisation

Résolution

Cas tests

I.a

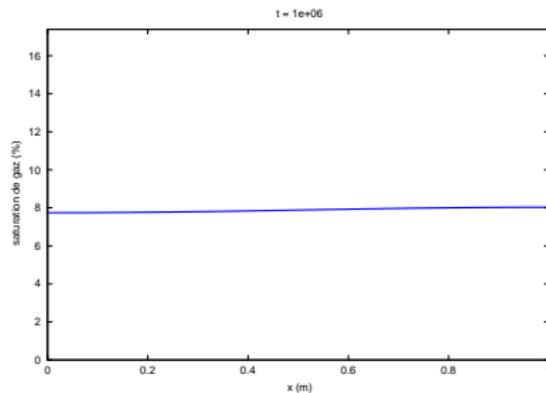
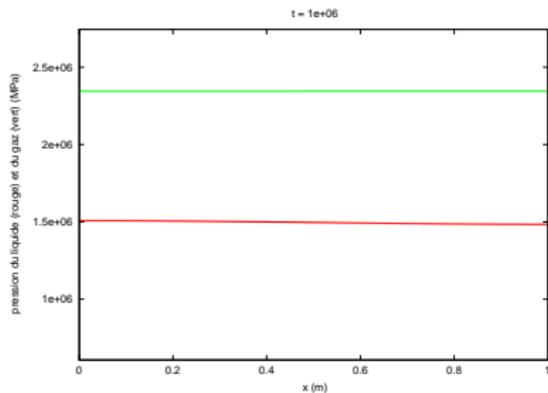
I.b

II.b

III.a

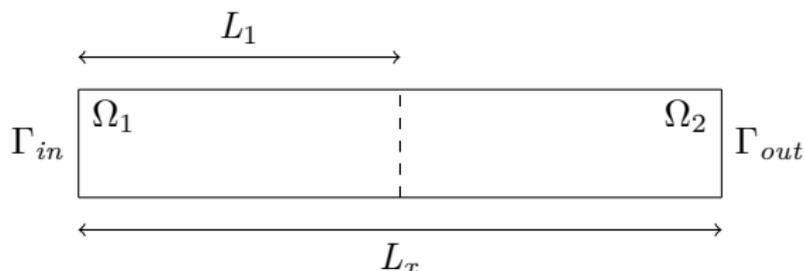
III.b

Propositions



# Propositions de cas tests

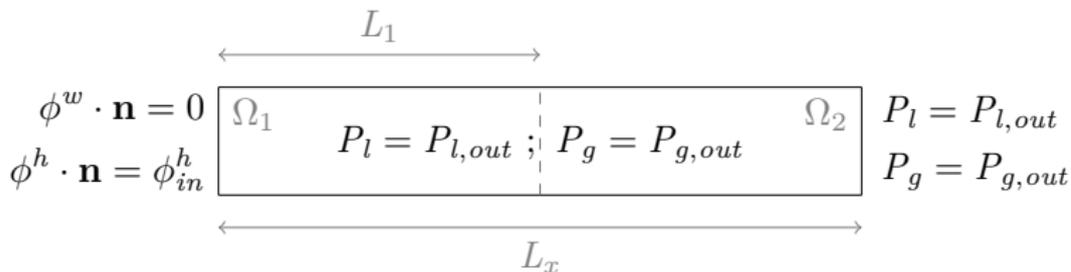
Pressions d'entrées : présentation



- ▶ Pression d'entrée :  $P_c(S_l = 1) = P_e > 0$
- ▶ Deux matériaux identiques sauf pressions d'entrée légèrement différentes
- ▶ Etat initial à l'équilibre
  - ▶  $S_g = 0$  à gauche
  - ▶  $S_g > 0$  à droite
- ▶ Injection d'hydrogène en  $\Gamma_{in}$

# Propositions de cas tests

Pressions d'entrées : présentation



Milieu poreux				Caractéristiques des fluides		
	$\Omega_1$	$\Omega_2$				
$k$	$10^{-16}$	$10^{-16}$	$m^2$	$D_l^h$	$3 \cdot 10^{-9}$	$m^2/s$
$\Phi$	0.3	0.3	(-)	$\mu_l$	$1 \cdot 10^{-3}$	$Pa \cdot s$
$P_e$	$2.1 \cdot 10^6$	$1.9 \cdot 10^6$	$Pa$	$\mu_g$	$9 \cdot 10^{-6}$	$Pa \cdot s$
$\lambda$	0.5	0.5	(-)	$H$	$7.65 \cdot 10^{-6}$	$mol/Pa/m^3$
$S_{lr}$	0	0	(-)	$M^w$	18	$g/mol$
$S_{gr}$	0	0	(-)	$M^h$	2	$g/mol$
				$\rho_l^{std}$	$10^3$	$kg/m^3$
				$T$	303	$K$

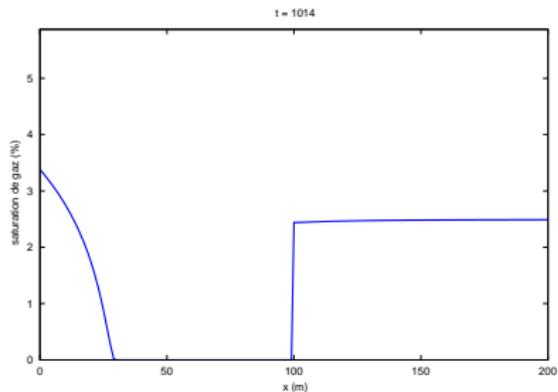
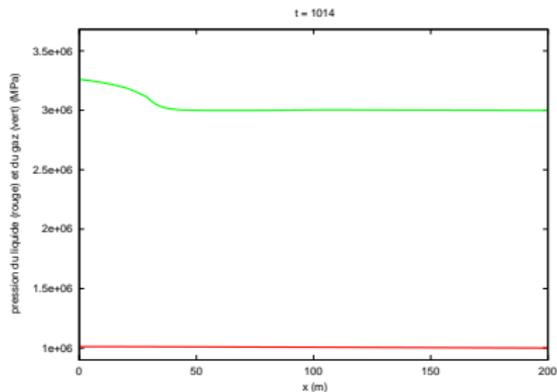
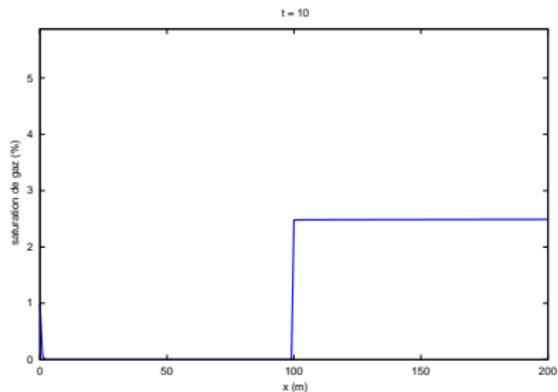
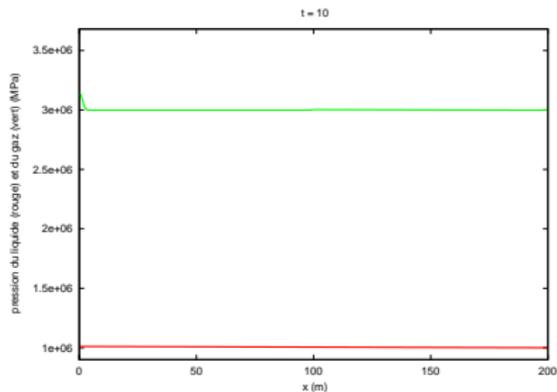
$L_x$	200	$m$
$L_1$	100	$m$
$Q^h$	500	$mg/m^2/ans$
$P_{l,out}$	$10^6$	$Pa$
$P_{g,out}$	$3 \cdot 10^6$	$Pa$
$T_{simul}$	$2 \cdot 10^4$	$ans$

$$p_c = P_e S_{le}^{-1/\lambda}, \quad k_{rl} = S_{le}^{(2+3\lambda)/\lambda} \quad \text{et} \quad k_{rg} = (1 - S_{le})^2 (1 - S_{le}^{(2+\lambda)/\lambda})$$

$$\text{avec} \quad S_{le} = \frac{S_l - S_{lr}}{1 - S_{lr} - S_{gr}}$$

# Propositions de cas tests

## Pressions d'entrées : simulation



# Propositions de cas tests

## Pressions d'entrées : simulation

Simulations des cas tests diphasiques  
MoMaS

Alain Bourgeat,  
Magdalena  
Dymitrowska, Farid  
Smaï

Modélisation

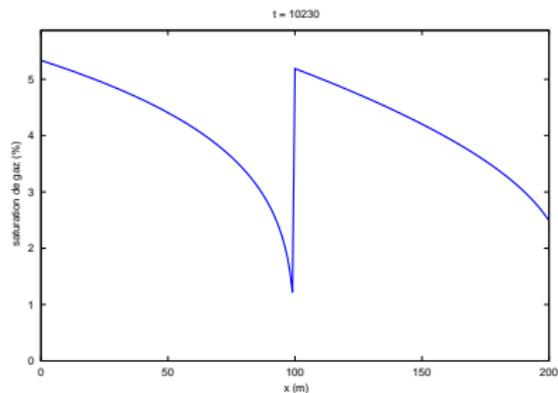
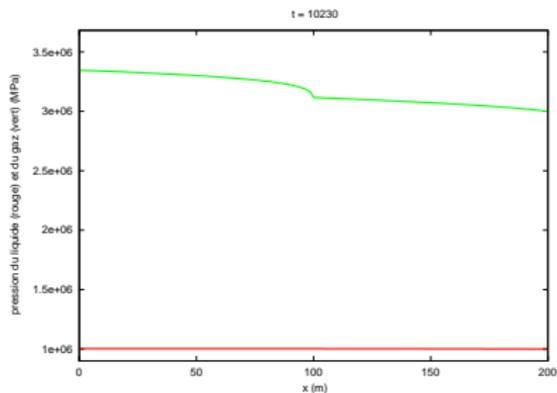
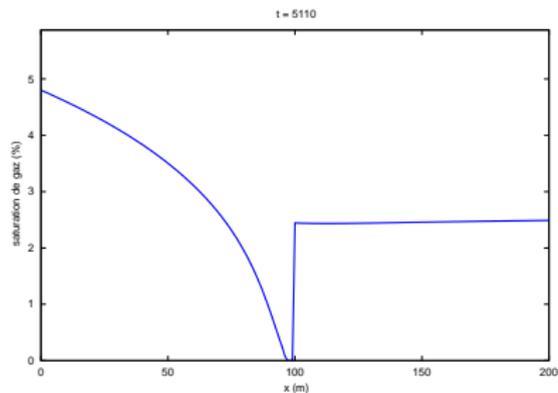
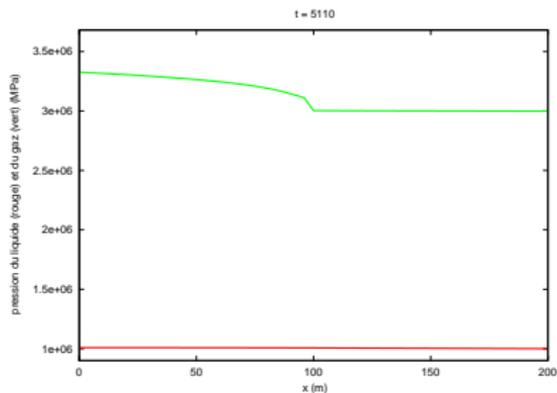
Résolution

Cas tests

Propositions

Pressions d'entrées

Effet du jeu



# Propositions de cas tests

Pressions d'entrées : simulation

Simulations des cas tests diphasiques MoMaS

Alain Bourgeat, Magdalena Dymitrowska, Farid Smaï

Modélisation

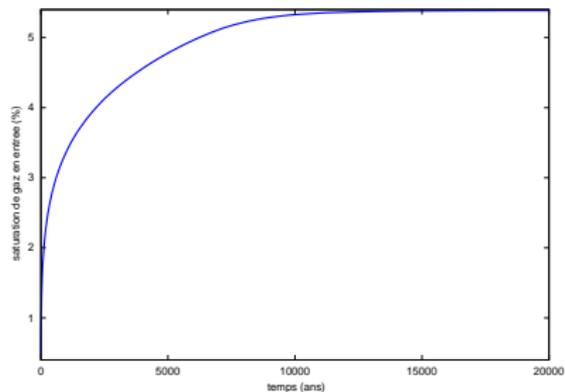
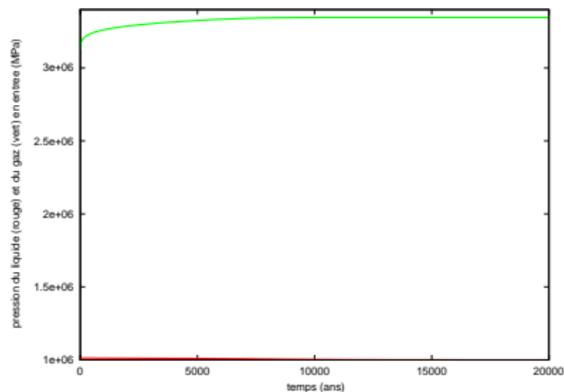
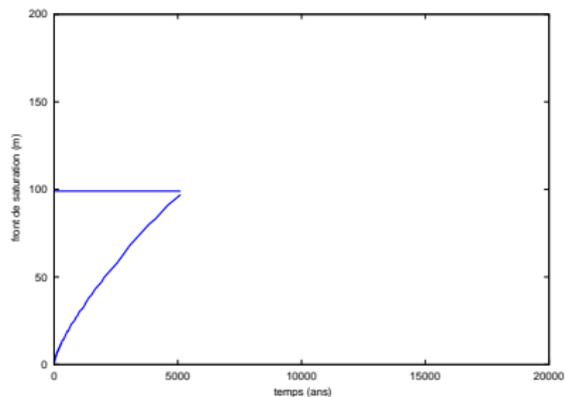
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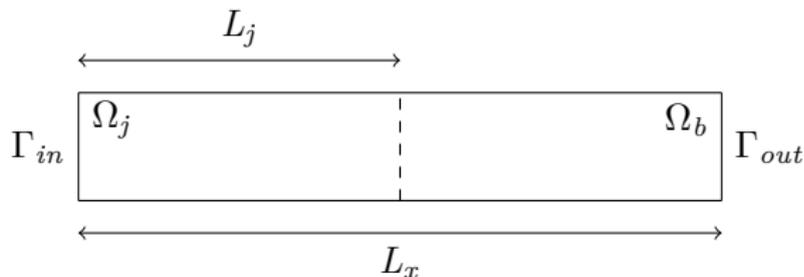
Pressions d'entrées

Effet du jeu



# Propositions de cas tests

Effet du jeu : présentation



- ▶ Modélisation du jeu par un milieu poreux
  - ▶ très perméable
  - ▶ très "facile" à désaturer
- ▶ Matériau propice à de fort écoulement
- ▶ Etat initial du jeu ?

# Propositions de cas tests

Effet du jeu : présentation

$$\begin{array}{c}
 \xleftarrow{L_j} \\
 \phi^w \cdot \mathbf{n} = 0 \\
 \phi^h \cdot \mathbf{n} = \phi_{in}^h \\
 \xleftarrow{L_x}
 \end{array}
 \begin{array}{|c|c|c|c|}
 \hline
 \Omega_j & P_l = P_{l,1} & P_l = P_{l,2} & \Omega_b \\
 \hline
 & P_g = P_{g,1} & x_l^h = 0 & \\
 \hline
 \end{array}
 \begin{array}{l}
 P_l = P_{l,2} \\
 x_l^h = 0
 \end{array}$$

Milieu poreux				Caractéristiques des fluides		
	$\Omega_j$	$\Omega_b$				
$k$	$10^{-12}$	$5 \cdot 10^{-17}$	$m^2$	$D_l^h$	$3 \cdot 10^{-9}$	$m^2/s$
$\Phi$	1	0.4	(-)	$\mu_l$	$1 \cdot 10^{-3}$	$Pa \cdot s$
$P_r$	$10^4$	$2 \cdot 10^6$	$Pa$	$\mu_g$	$9 \cdot 10^{-6}$	$Pa \cdot s$
$n$	4	1.5	(-)	$H$	$7.65 \cdot 10^{-6}$	$mol/Pa/m^3$
$S_{lr}$	0	0.4	(-)	$M^w$	18	$g/mol$
$S_{gr}$	0	0	(-)	$M^h$	2	$g/mol$
				$\rho_l^{std}$	$10^3$	$kg/m^3$
				$T$	303	$K$

$L_x$	10	$m$
$L_j$	2	$m$
$Q^h$	200	$mg/m^2/ans$
$P_{l,1}$	$8 \cdot 10^4$	$Pa$
$P_{g,1}$	$10^5$	$Pa$
$P_{l,2}$	$10^6$	$Pa$
$T_{simul}$	$10^6$	$ans$

$$p_c = P_r \left( S_{le}^{-1/m} - 1 \right)^{1/n}, \quad kr_l = \sqrt{S_{le}} \left( 1 - (1 - S_{le}^{1/m})^m \right)^2 \quad \text{et} \quad kr_g = \sqrt{1 - S_{le}} \left( 1 - S_{le}^{1/m} \right)^{2m}$$

avec  $S_{le} = \frac{S_l - S_{lr}}{1 - S_{lr} - S_{gr}}$  et  $m = 1 - \frac{1}{n}$

# Propositions de cas tests

## Effet du jeu : simulation

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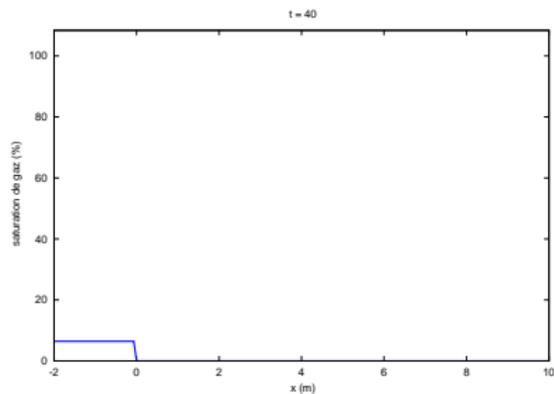
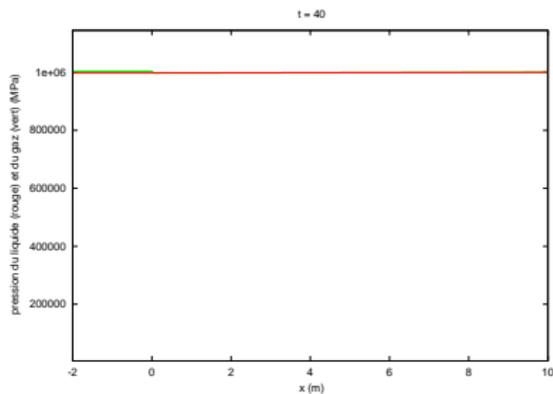
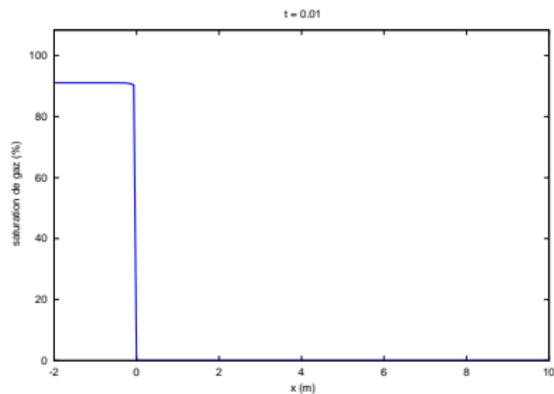
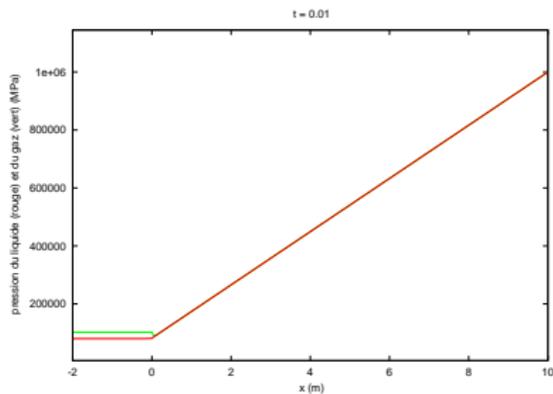
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# Propositions de cas tests

## Effet du jeu : simulation

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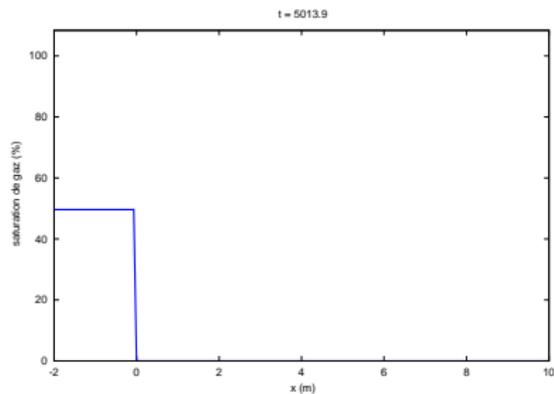
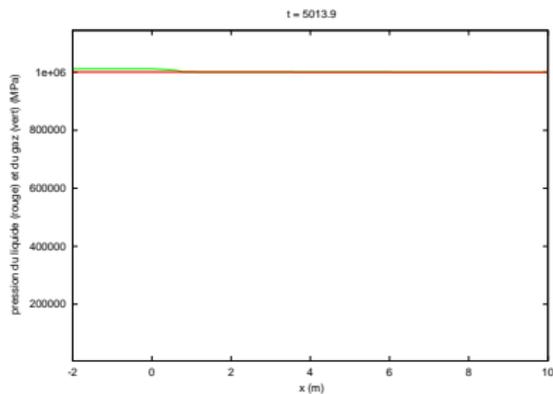
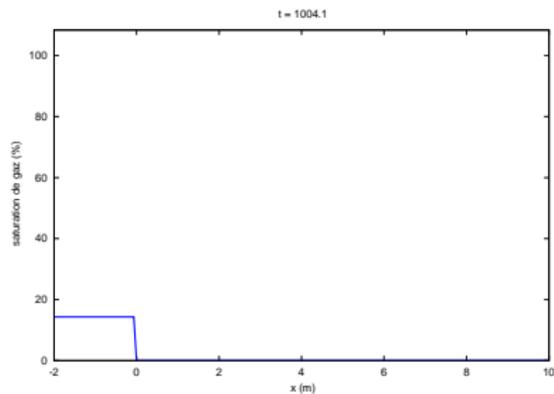
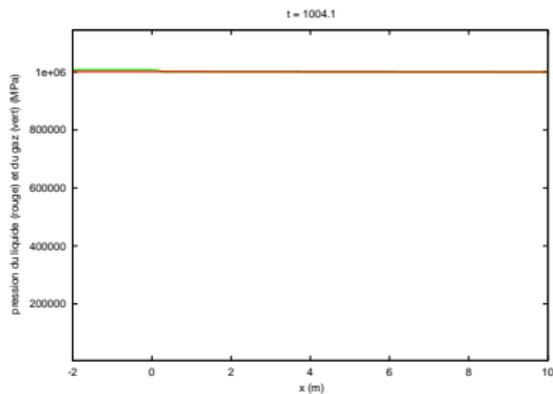
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# Propositions de cas tests

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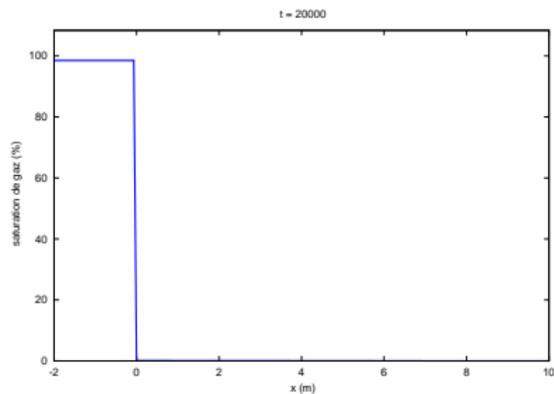
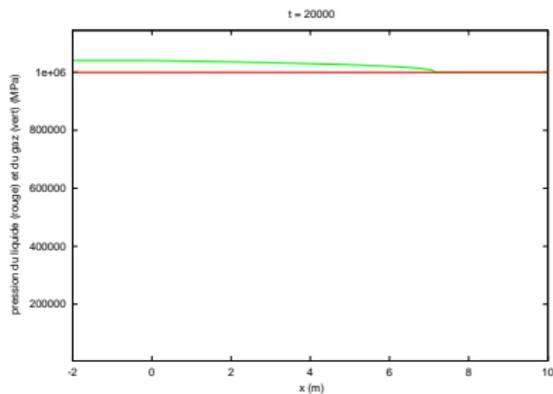
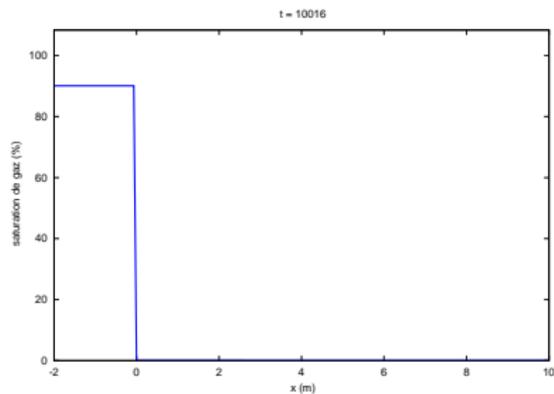
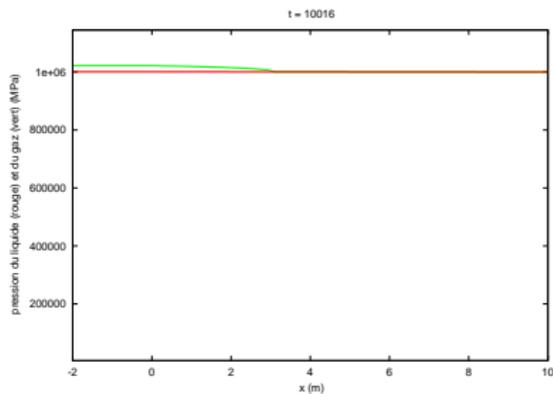
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Effet du jeu : simulation

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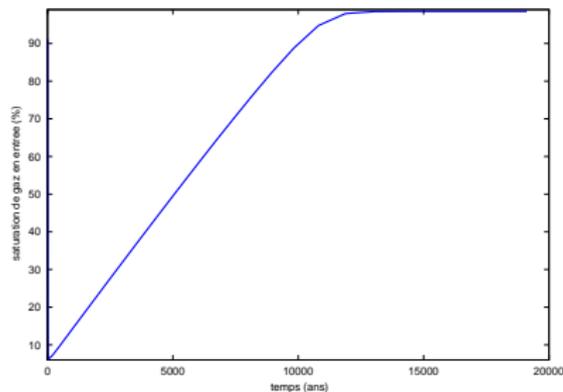
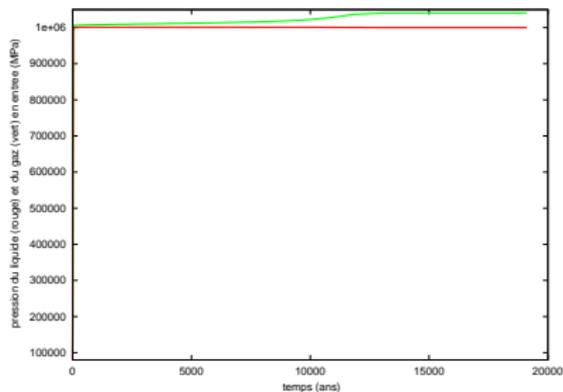
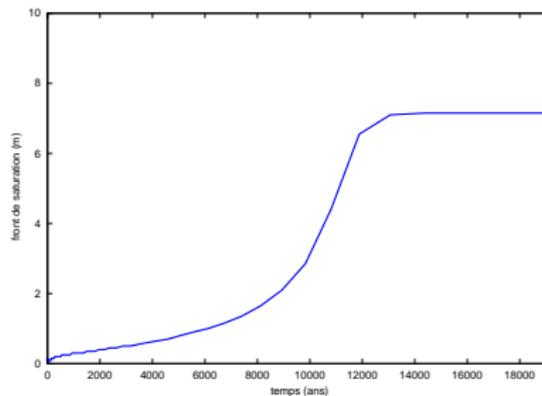
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Effet du jeu



- ▶ L'effet de la vapeur d'eau n'est pas toujours négligeable
  - ▶ peut faciliter l'apparition du gaz
  - ▶ augmente le transport du gaz (diffusion dans le gaz élevée)
  
- ▶ Peut-on toujours se restreindre à 2 composants ?