COMSOL
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AMPHOS 21
SCIENTIFIC AND STRATEGIC ENVIRONMENTAL CONSULTING

Two-phase flow models of gas generation and transport in geological formations

Orlando Silva
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Outline

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- ☐ Objectives
- ☐ Modeling Approach
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    - Implementation in Comsol
- ☐ Verification examples
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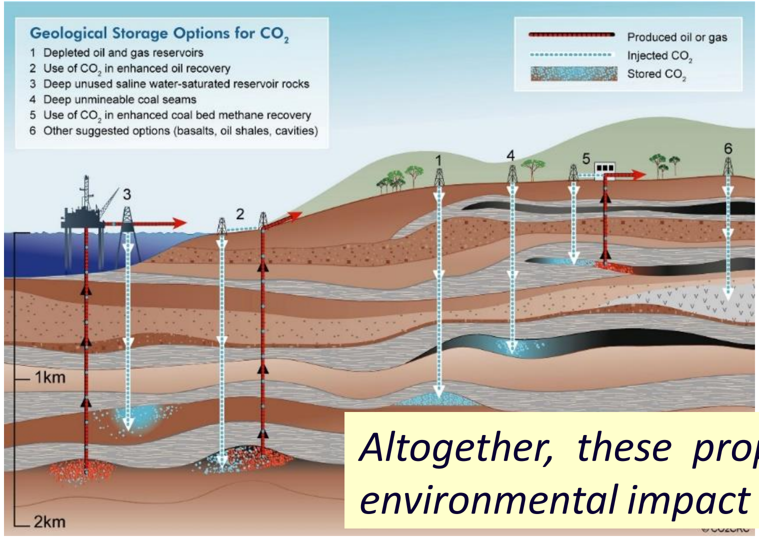
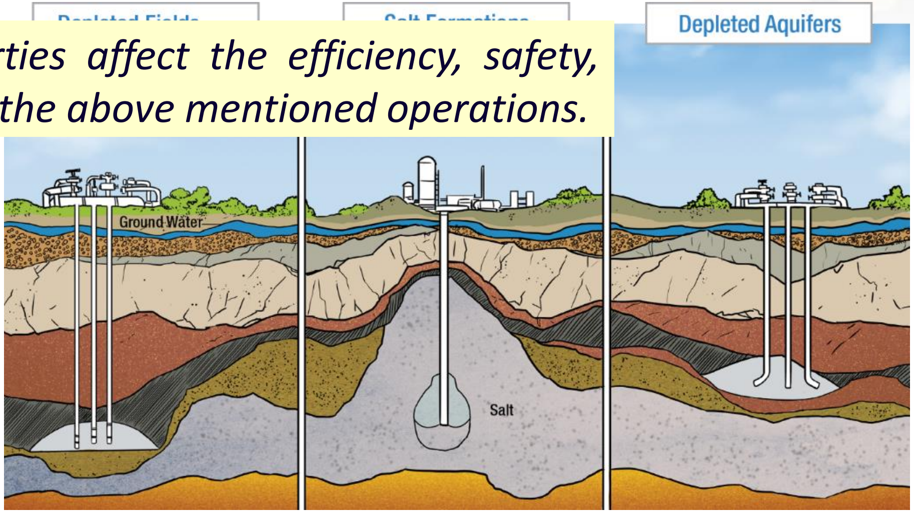
- ☐ Application example
- ☐ Conclusions

Context



Gas phase evolution depends on the thermodynamic conditions at depth, the properties of the fluids (density, viscosity, surface tension) and the geological formation (permeability, porosity, retention curve), and the chemical interaction between fluids and solid (e.g., minerals, concrete, steel).

Altogether, these properties affect the efficiency, safety, environmental impact of the above mentioned operations.



Gas generation and transport through porous media is a process common to many field applications such as radioactive waste and underground gas storage.

Objectives

The objectives of this work are

- ☐ To implement in Comsol Multiphysics both miscible and immiscible two-phase flow models in porous media.
- ☐ To apply these models to simulate the evolution of gases in geological formations.

Governing equations

Miscible compositional approach

$$\frac{\partial C_T^k}{\partial t} = -\nabla\cdot\left(\mathbf{J}_l^k + \mathbf{J}_g^k + \mathbf{q}^k C_l^k\right) + Q_l^k + Q_g^k$$

$$C_T^k = \phi S_l C_l^k + \phi S_g C_g^k + (1-\phi) C_s^k$$

$$\mathbf{q}_i = -\frac{\mathbf{k} k_{ri}}{\mu_i}\left(\nabla P_i + \rho_i g \mathbf{z}\right)$$

$$\mathbf{q}^k = \mathbf{q}_l + \mathbf{q}_g H_{gl}^k$$

$$\mathbf{J}_i^k = -\phi S_i \mathbf{D}_i^k \nabla C_i^k$$

Immiscible two-phase flow

$$\phi\rho_g \frac{\partial S_g}{\partial t} + \nabla\cdot\left(-\mathbf{k}\lambda_g\rho_g\nabla P_l - \mathbf{k}\lambda_g\rho_g\frac{\partial P_c}{\partial S_g}\nabla S_g - \mathbf{k}\lambda_g\rho_g^2 g\mathbf{z}\right) + \frac{\partial(\phi\rho_g)}{\partial t} S_g = \sum_{k=1}^{N_c} Q_g^k$$

$$\phi(\rho_g-\rho_l)\frac{\partial S_g}{\partial t} + \nabla\cdot\left(-\mathbf{k}(\lambda_g\rho_g+\lambda_l\rho_l)\nabla P_l - \mathbf{k}\lambda_g\rho_g\frac{\partial P_c}{\partial S_g}\nabla S_g - \mathbf{k}(\lambda_g\rho_g^2+\lambda_l\rho_l^2)g\mathbf{z}\right) + \frac{\partial(\phi(\rho_g-\rho_l))}{\partial t} S_g = -\frac{\partial(\phi\rho_l)}{\partial t} + \sum_{k=1}^{N_c}\left(Q_l^k + Q_g^k\right)$$

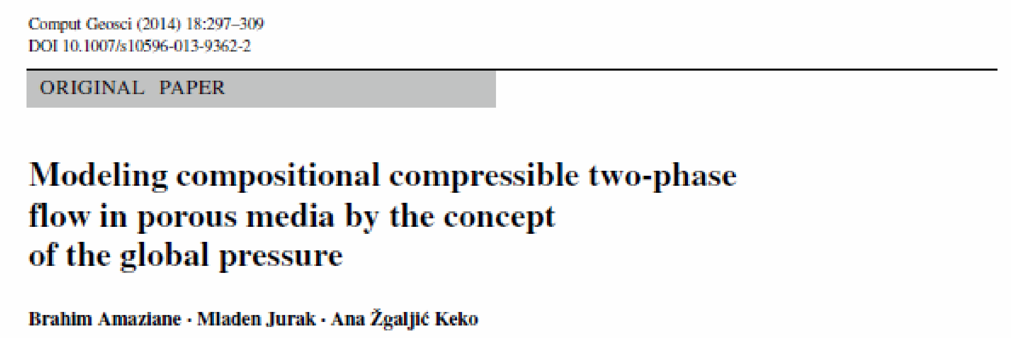
COMSOL implementation

Using the **coefficient's form of the PDE module** with multiple dependent variables

$$\boxed{\mathbf{e_a}\frac{\partial^2\mathbf{u}}{\partial t^2} + \mathbf{d_a}\frac{\partial\mathbf{u}}{\partial t} - \nabla\cdot\left(\mathbf{c}\nabla\mathbf{u} + \boldsymbol{\alpha}\mathbf{u} - \boldsymbol{\gamma}\right) + \boldsymbol{\beta}\cdot\nabla\mathbf{u} + \mathbf{a}\mathbf{u} = \mathbf{f}}$$

Verification examples

- The miscible formulation was verified with a 1D problem for testing the ability of codes to simulate the gas phase appearance and disappearance including gas solubility (Amaziane et al., 2014).



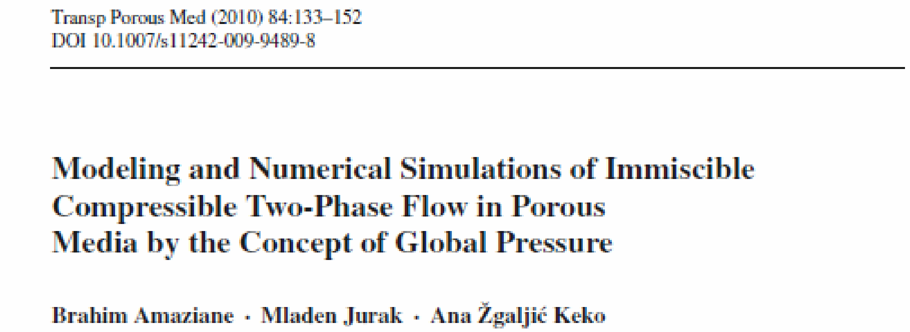
Comput Geosci (2014) 18:297–309
DOI 10.1007/s10596-013-9362-2

ORIGINAL PAPER

Modeling compositional compressible two-phase flow in porous media by the concept of the global pressure

Brahim Amaziane · Mladen Jurak · Ana Žgaljić Keko

- The immiscible approach was verified with three 1D examples neglecting gravity effects (Amaziane et al., 2010).



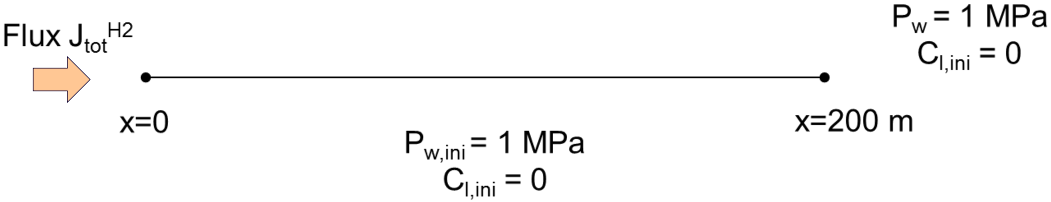
Transp Porous Med (2010) 84:133–152
DOI 10.1007/s11242-009-9489-8

Modeling and Numerical Simulations of Immiscible Compressible Two-Phase Flow in Porous Media by the Concept of Global Pressure

Brahim Amaziane · Mladen Jurak · Ana Žgaljić Keko

Verification of miscible approach

The benchmark example considers an isothermal liquid-gas system with two components with properties close to water and hydrogen.



Flux J_{tot}^{H2}

$P_w = 1$ MPa
$C_{l,ini} = 0$

x=0

x=200 m

$P_{w,ini} = 1$ MPa
$C_{l,ini} = 0$

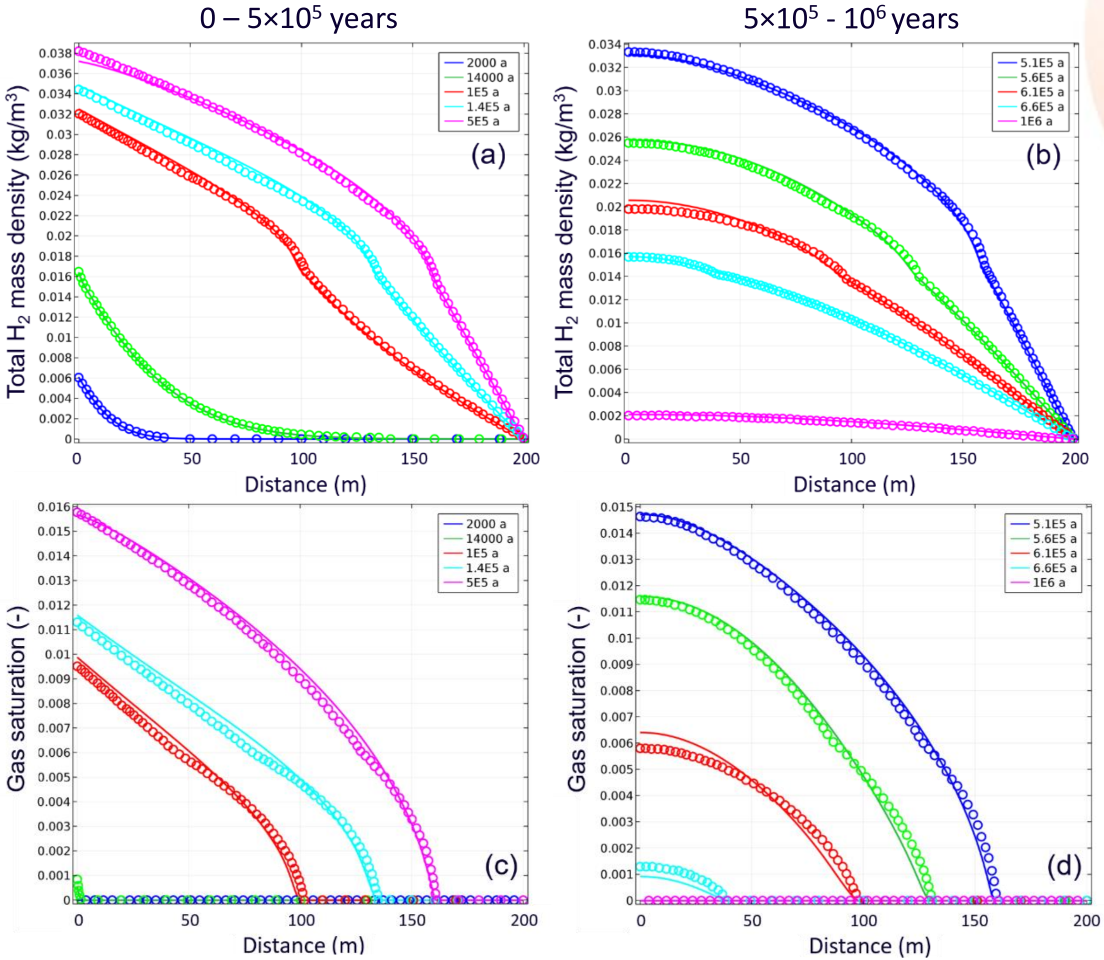
- **Constitutive relationships** were implemented as local equations by using Comsol variables:
  - System at 30 ºC
  - Constant liquid density and viscosity, gas viscosity, molecular diffusion of hydrogen in the liquid and Henry constant of hydrogen
  - No water evaporation
  - Retention and permeability functions according to the van Genuchten model (1980)
  - Hydrogen is injected on the left boundary into the domain for the first 5×10^5 years at a rate of 5.57×10^{-6} kg/year

- **Solver.** The system of equations was solved with the MUMPS (MUltifrontal Massively Parallel sparse direct Solver) solver available in COMSOL, using an iterative Newton-Raphson method, estimating time derivatives with a BDF (Backward Differentiation Formula) solver, and discretizing the 1D domain into 200 Lagrange elements of second order.

Gas appearance and disappearance

$$X = C_T^k / \phi = S_l C_l^{H_2} + S_g C_g^{H_2}$$

A change in the slope of the total hydrogen concentration profile is associated to the gas front position

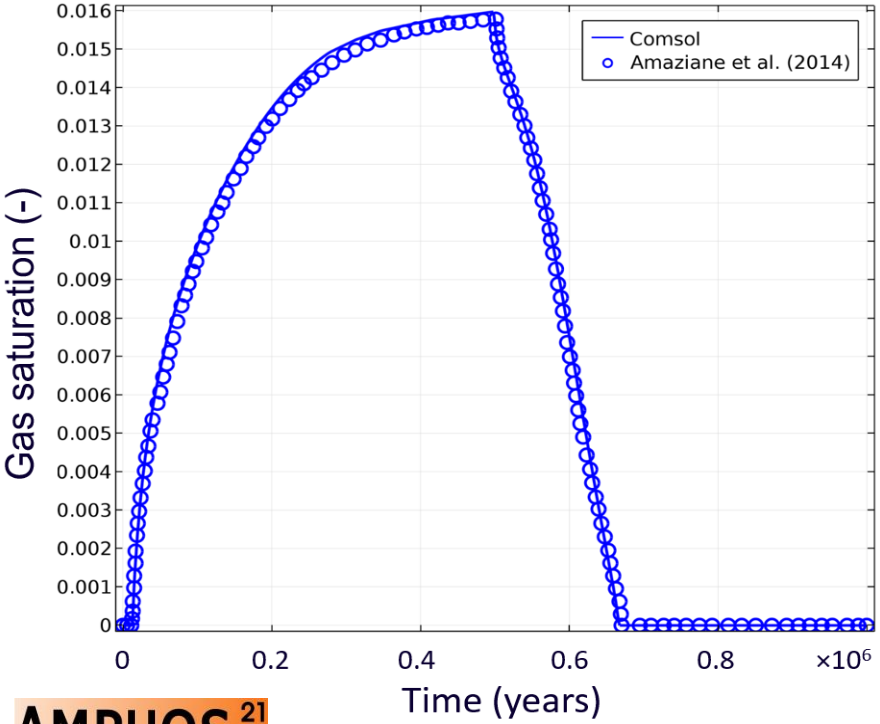


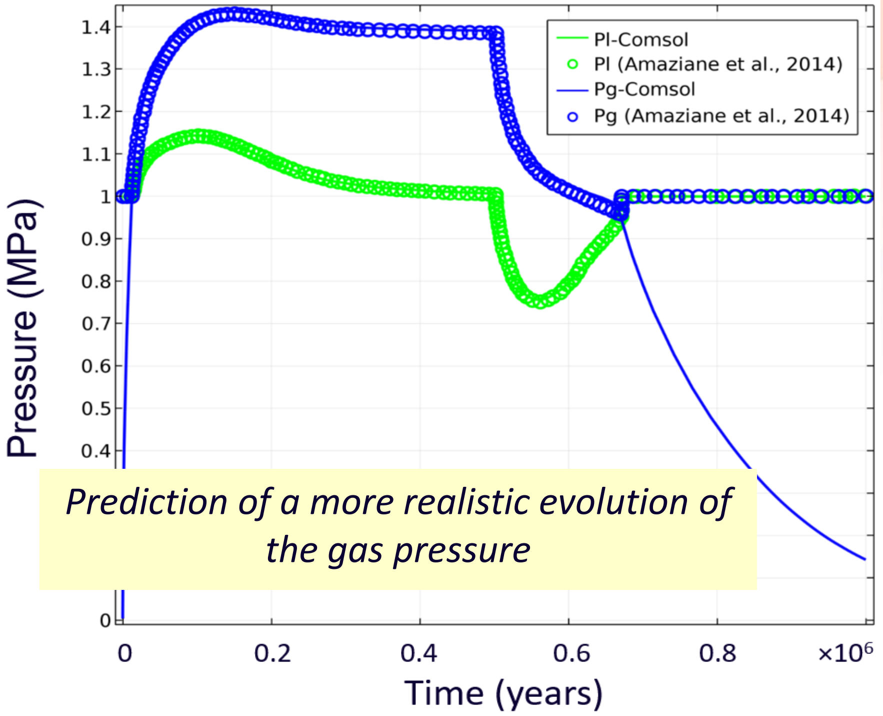
0 – 5×10^5 years

5×10^5 - 10^6 years

Gas appearance and disappearance

Gas saturation and pressures at the inlet boundary





Prediction of a more realistic evolution of the gas pressure

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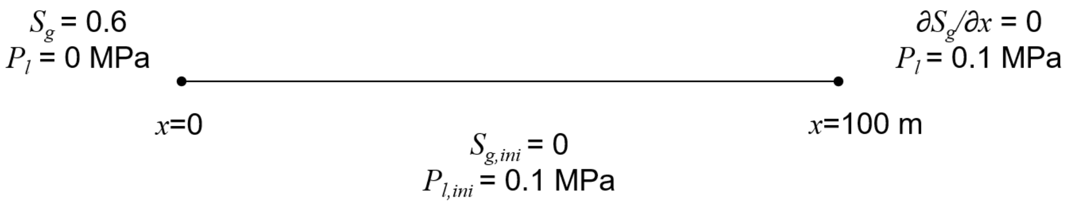
Verification of immiscible approach 1



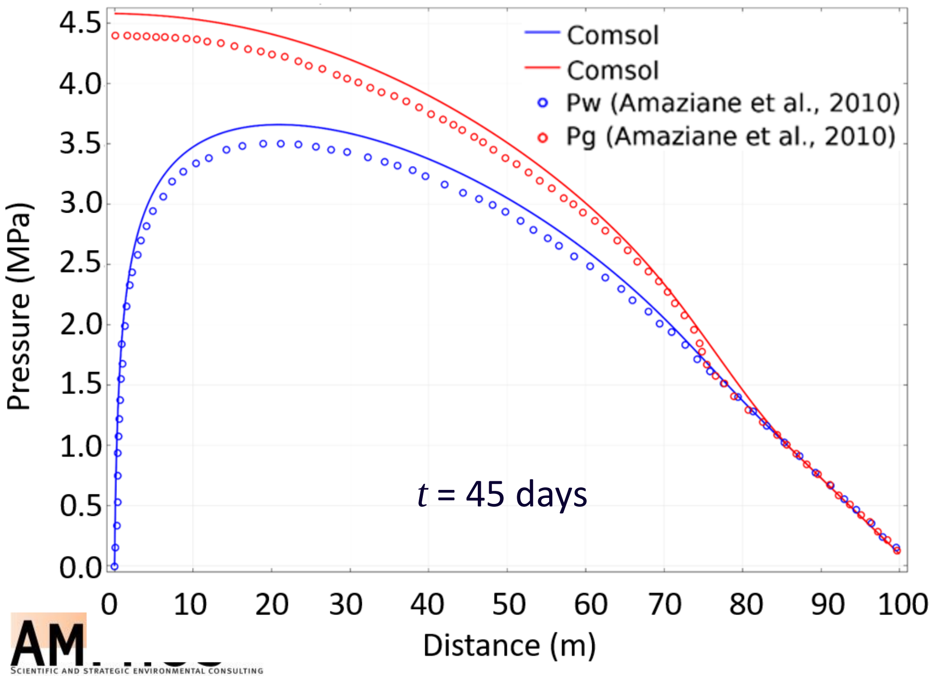
S_g = 0.6
P_l = 0 MPa

$\partial S_g/\partial x$ = 0
P_l = 0.1 MPa

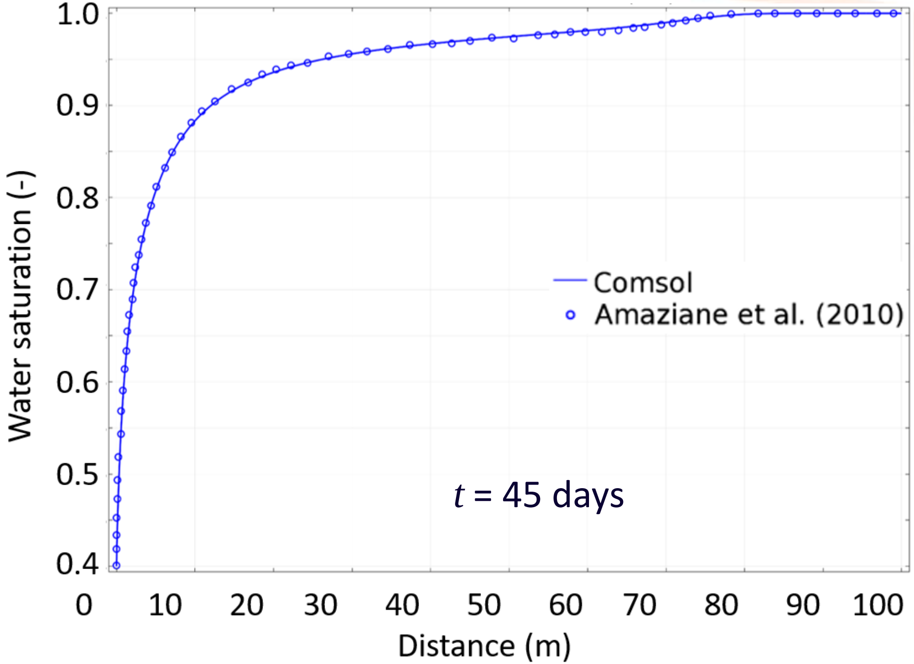
x=0

x=100 m

$S_{g,ini}$ = 0
$P_{l,ini}$ = 0.1 MPa

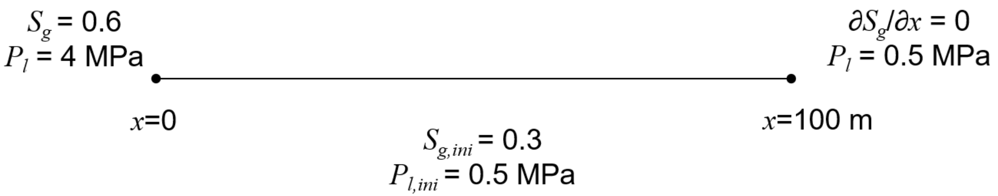


t = 45 days



t = 45 days

Verification of immiscible approach 2



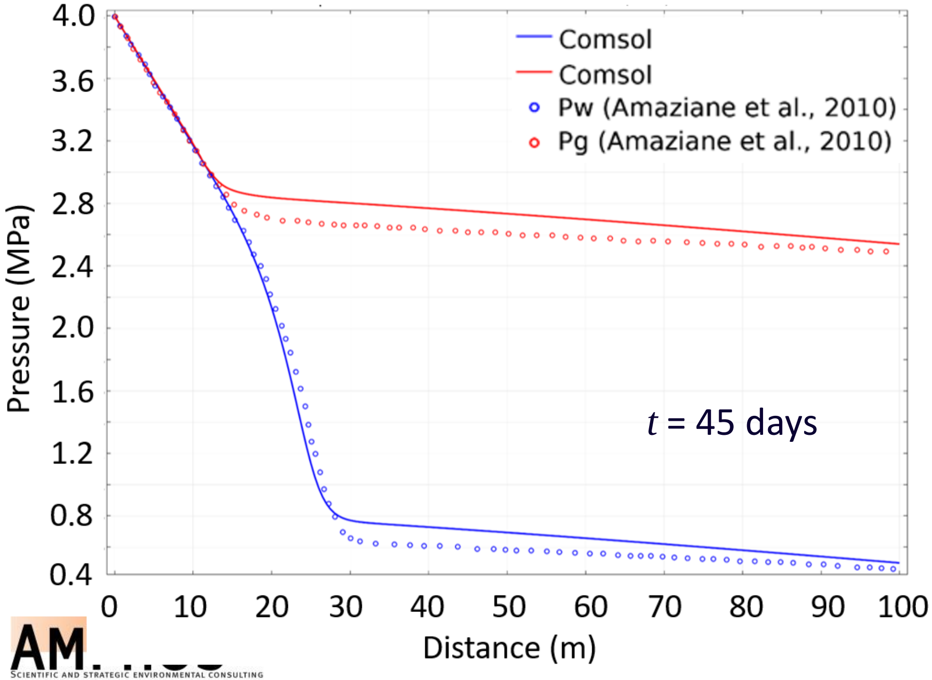
S_g = 0.6
P_l = 4 MPa

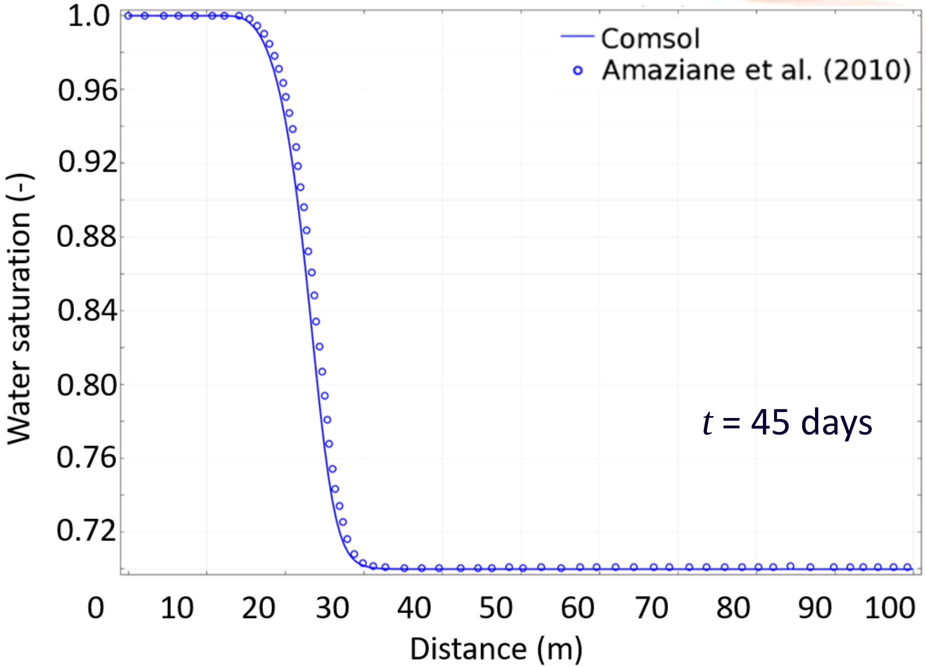
x=0

$\partial S_g/\partial x$ = 0
P_l = 0.5 MPa

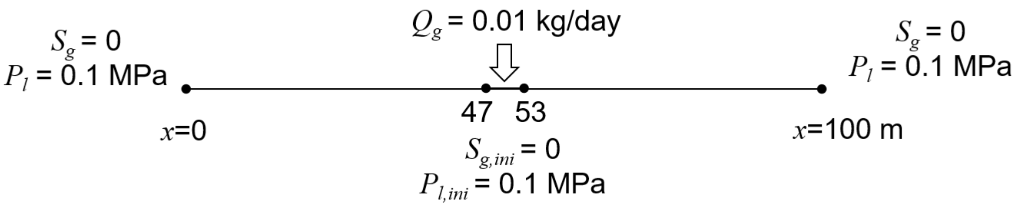
x=100 m

$S_{g,ini}$ = 0.3
$P_{l,ini}$ = 0.5 MPa





Verification of immiscible approach 3



S_g = 0
P_l = 0.1 MPa

Q_g = 0.01 kg/day

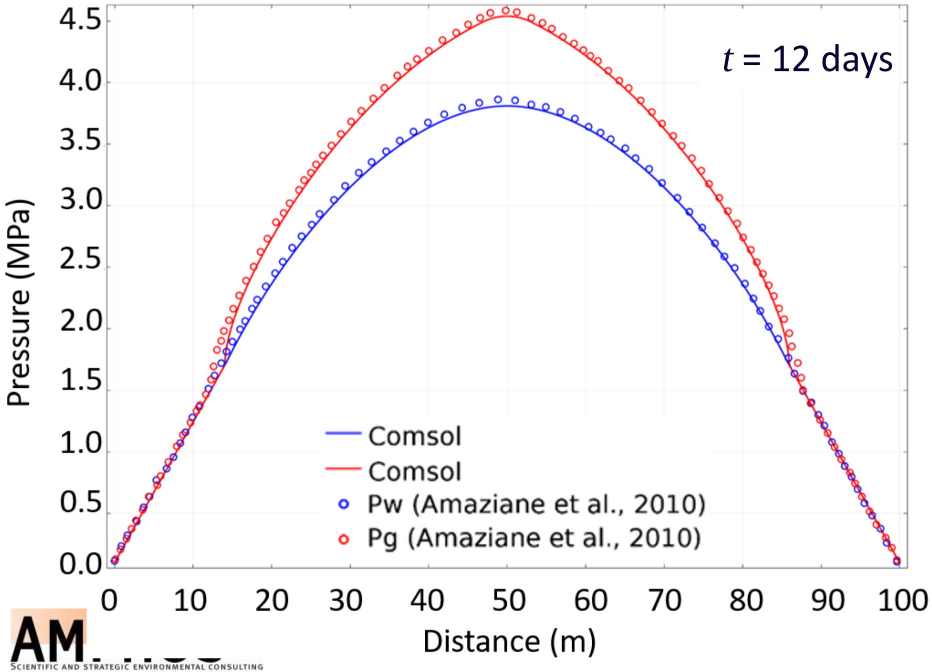
S_g = 0
P_l = 0.1 MPa

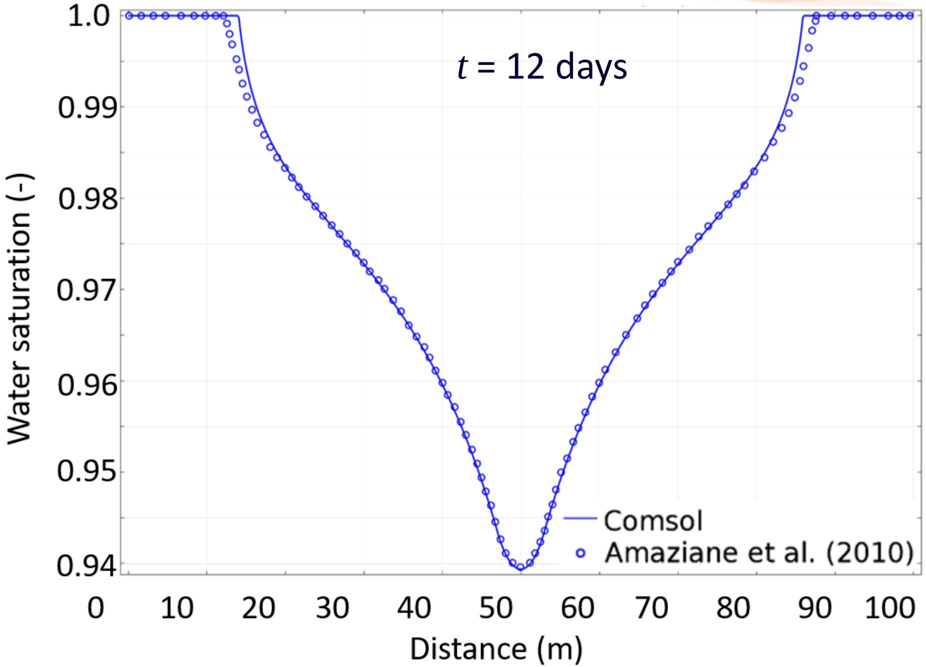
x=0

47 53

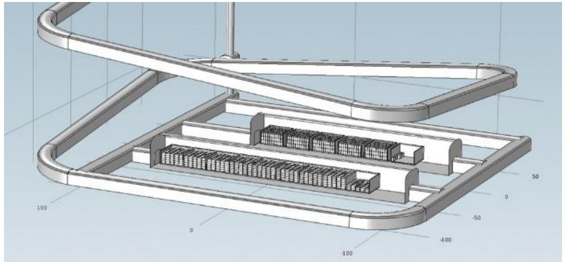
x=100 m

$S_{g,ini}$ = 0
$P_{l,ini}$ = 0.1 MPa

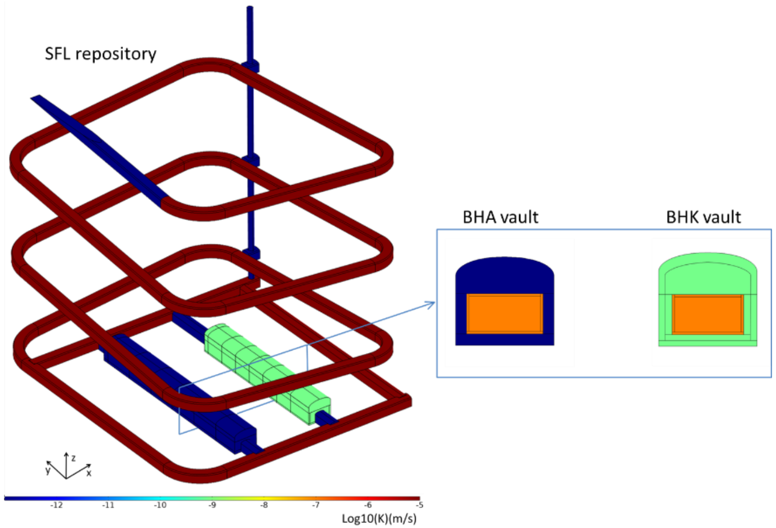


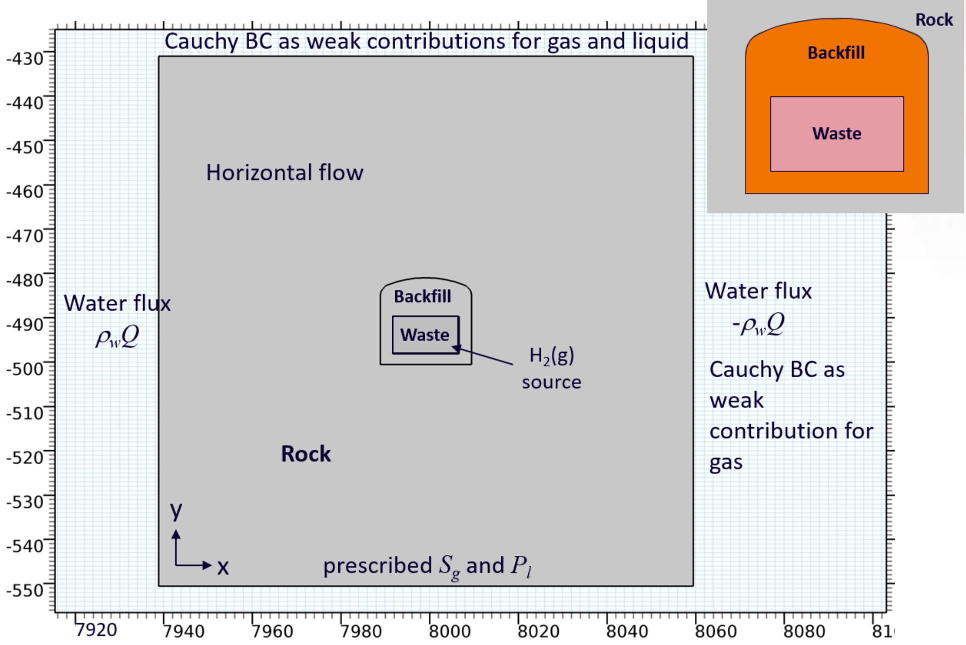


Application. Radionuclide waste storage

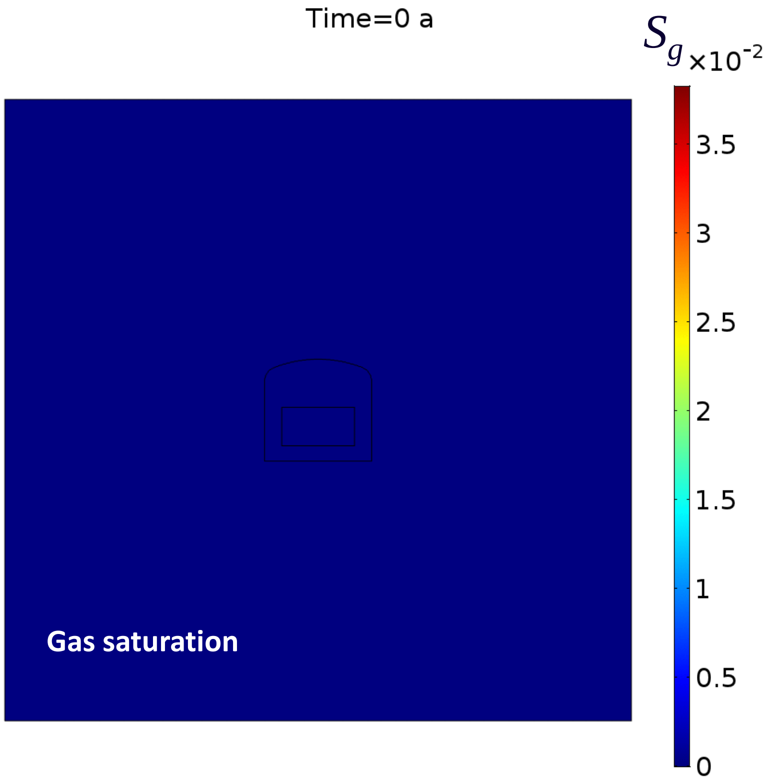


H_2(g) is generated in the waste compartment due to steel corrosion

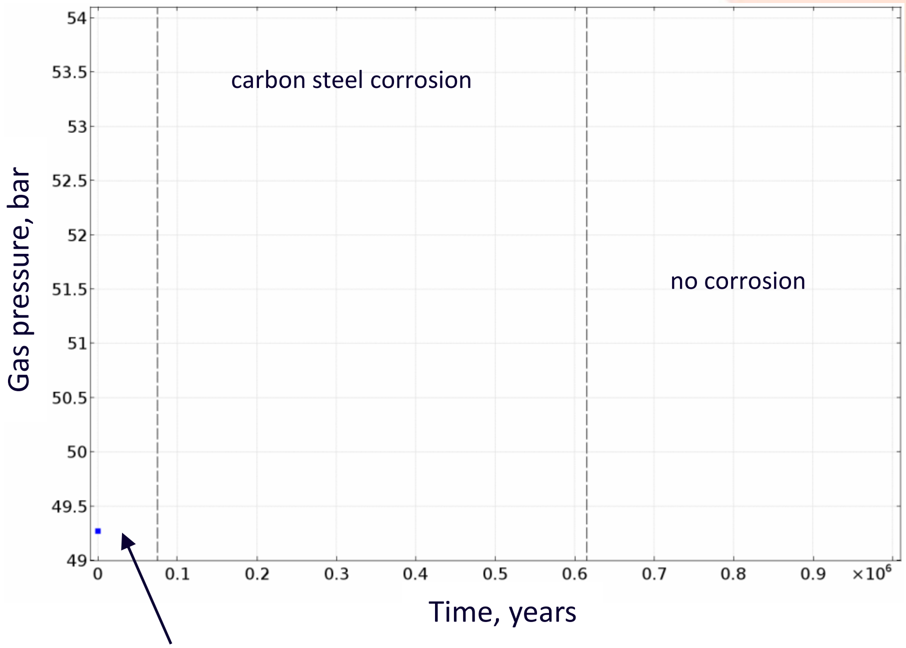




Application. Radionuclide waste storage



Average gas pressure in the vault



carbon steel corrosion

no corrosion

stainless & carbon steel corrosion

Conclusions

- ☐ Miscible and immiscible two-phase flow formulations were implemented in Comsol Multiphysics 5.2a and verified with published benchmarks.
- ☐ The present miscible approach predicts a more realistic evolution of the gas pressure than other miscible approaches.
- ☐ The present two-phase flow approaches are able to describe gas generation and transport under miscible and immiscible conditions. Which approach is more practical or advantageous depends on the specific application.

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ESPAÑA
Paseo de García Faria, 49-51
08019 Barcelona
Tel.: +34 93 583 05 00

Paseo de la Castellana 40, 8ª Planta
28046 Madrid
Tel.: +34 620634729

CHILE
Avda. Nueva Tajamar, 481
WTC – Torre Sur – Of 1005
Las Condes, Santiago
Tel.: +562 2 7991630

PERÚ
Jr. Pietro Torrigiano 396
San Borja, Lima 41
Tel.: +51 1 592 1275

FRANCE
92 Rue du Sergent Blandan
54000 Nancy
Tel.: +33 645 766 322