Coupled Two-Phase Flow

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Outline

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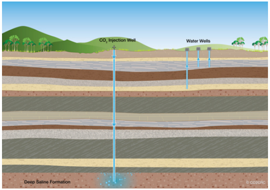
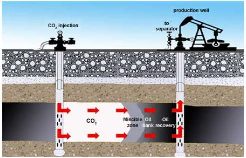
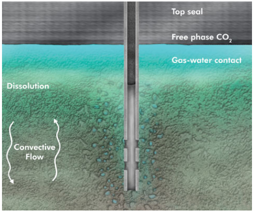
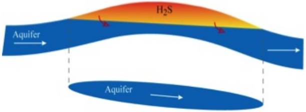






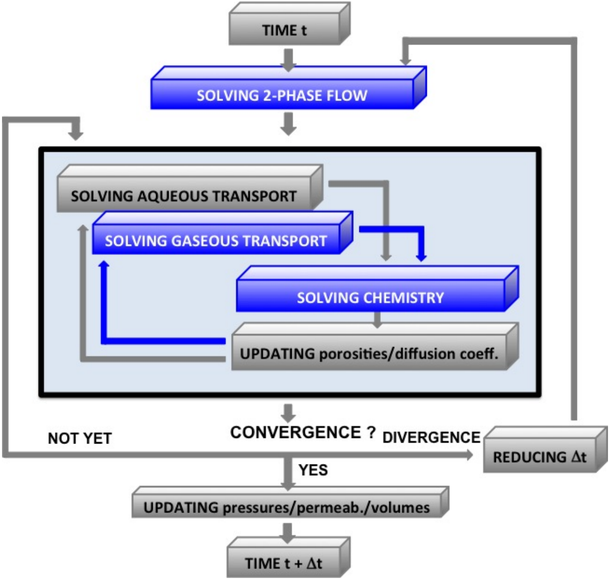


Bonnaud et al. 2012

Objectives

- The development of a Two-Phase Flow module in the reactive transport software HYTEC.
- The prospective applications : H2S leaching in acid gas reservoir in contact with active aquifer and an experiment MIRAGES carried out at the University of Lorraine.

HYTEC software



Two-Phase Multicomponent Reactive Transport Model

Coupled Fully Implicit or Operator-Splitting ?
Sequential Partly Iterative :

- Resolve firstly two-phase flow (also saturated or unsaturated regime is available), $\alpha = \{l, g\}$

$$\frac{\partial \omega \rho_\alpha S_\alpha}{\partial t} = \mathfrak{F}\left(S_\alpha, p_\alpha\right) + R_\alpha$$

- Iterate transport and chemistry operators until the convergence :

$$\begin{aligned} \frac{\partial \omega S_l c_i^l}{\partial t} &= \mathfrak{T}^l\left(c_i^l\right) + R_i^l\left(c_i^l, \bar{c}_i^l\right) \\ \frac{\partial \omega S_g c_i^g}{\partial t} &= \mathfrak{T}^g\left(c_i^g\right) + R_i^g\left(c_i^g\right) \\ c_i^\alpha &= \mathfrak{R}\left(c_i^{tot}\right) \end{aligned}$$

c_i - total mobile concentration of basis species,
$\bar{c}_i$ - immobile concentration,
$c_i^{tot} = c_i + \bar{c}_i$ - total concentration

Mathematical Model

- Mass conservation equations

$$\frac{\partial \omega \rho_\alpha S_\alpha}{\partial t} + \mathrm{div}(\rho_\alpha \overrightarrow{u_\alpha}) - \rho_\alpha q_\alpha = 0$$

- Darcy's velocities

$$\overrightarrow{u_\alpha} = -\frac{k_{r\alpha}}{\mu_\alpha} K \left(\overrightarrow{\mathrm{grad}} p_\alpha - \rho_\alpha \overrightarrow{g} \right)$$

- Closure laws

$$\begin{aligned} S_l + S_g &= 1 \\ p_g - p_l &= p_c(S_l) \end{aligned}$$

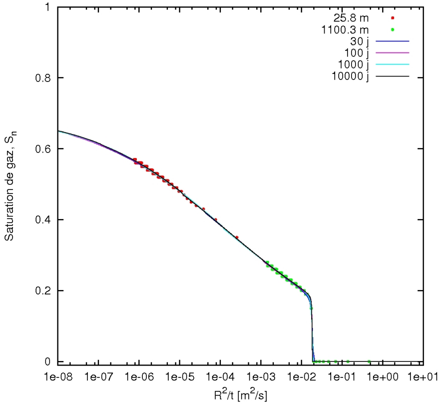
- primary variables : p_l, S_g
- non-linear functions $k_{r\alpha}$, p_c : modified Brooks-Corey (1954), van Genuchten(1980) models ($C^1([0,1])$).

Numerical Model

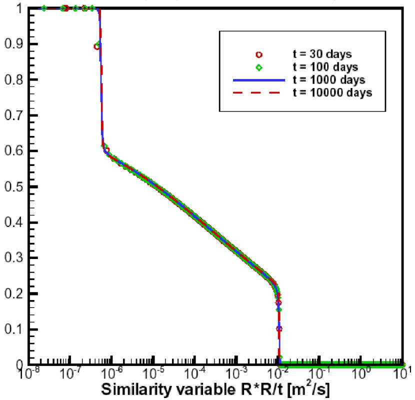
- Integral Finite Difference Method
- Spatial discretization : Two-Point Flux Approximation, mobility upwinding
- Time discretization : Implicit Euler, adaptive variable time step as advantage
- Jacobian resolution : analytical
- Resolution of linearized system :
  - ILU0, GMRES, additional preconditioner on the diagonal blocks
  - Newton –Raphson, max iteration number = 9
- Simplifications : isotropy

Test Case : 1D Radial Flow from a CO_2 Injection Well (Pruess, 2002)

Simulated gas saturation as a function of similarity variable R^2/t (Barenblatt, 1952)



HYTEC

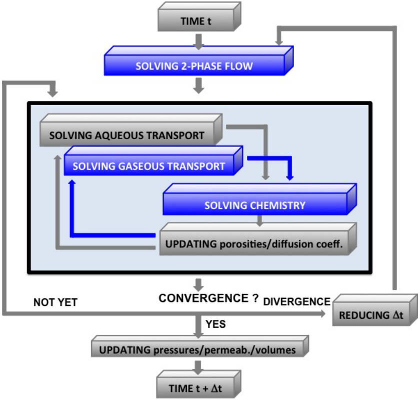


TOUGH2-ECO2 (Pruess, 2002)

- $R^2/t \leq 5\text{x}10^{-7}\ m^2/s$ - dry-out zone simulated by TOUGH2. HYTEC : $S_l \neq 0$
- $R^2/t < 2\text{x}10^{-2}\ m^2/s$ - two-phase state
- $R^2/t \geq 2\text{x}10^{-2}\ m^2/s$ - single-phase liquide state

Sequential Approach

- Separate resolution of two-phase flow allows to find the pressures p_α, the velocities $\overrightarrow{u_\alpha}$, the saturations S_α.
- The given information is used to solve the reactive transport that iterates until the *good* concentrations c_i. If not the two-phase flow is repeated with reduced time step.



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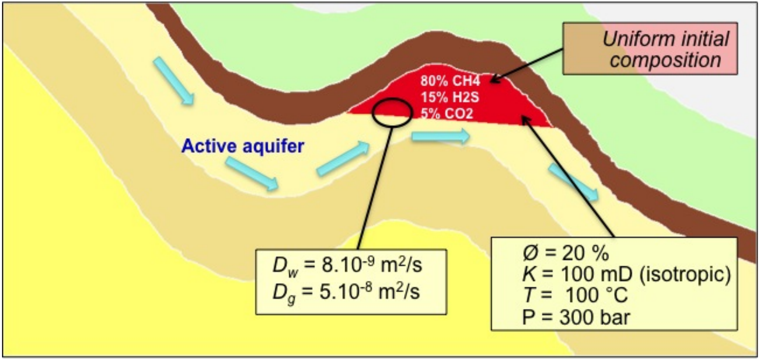
Numerical Results. Context of H_2S leaching.

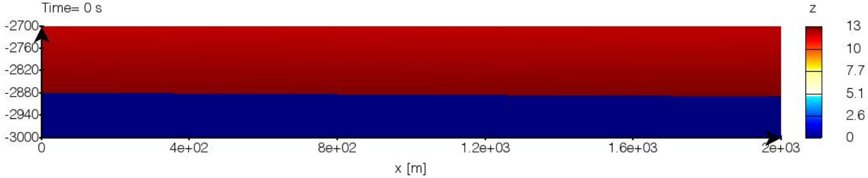
H_2S is colorless, flammable, soluble, corrosive and extremely toxic ; it can be found in gas/oil field, landfills, waste treatment plants. H_2S in natural gas reservoirs is also an important factor of economic depreciation even at very low concentration for oil and gas industry.



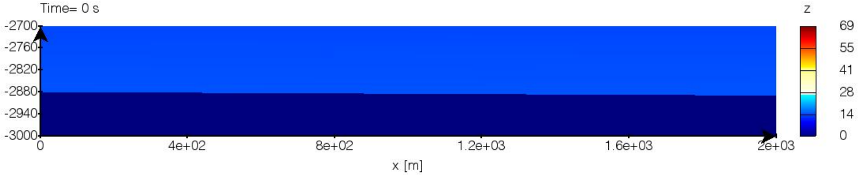
- H_2S and CO_2 are more soluble than CH_4 under conditions of pressure and temperature of a reservoir.
- Preferential leaching of H_2S in contact with an active aquifer is expected. (Bonnaud, 2012)

Preferential leaching of H_2S

Case 1 : Zero permeability in reservoir, $K_{abs} = 0$. There is only diffusive transport in gas phase. It is equivalent to a simulation with non-saturated model in the work of Bonnaud, 2012.



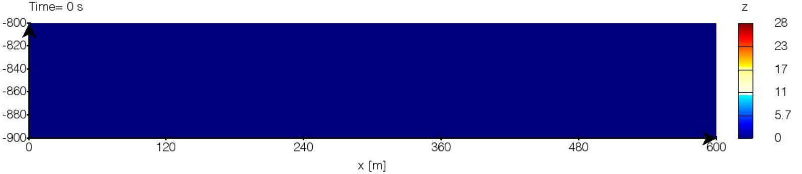
Case 2 : Full two-phase flow :



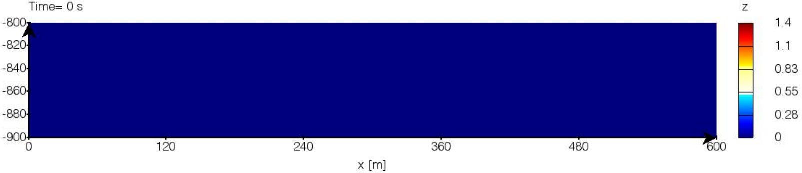
H_2S, molal

CO_2 injection in a fully water-saturated domain (2D). (Neumann, 2012)

$CO_{2(g)}$, molal



$CO_{2(aq)}$, molal



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CO_2 injection in a fully water-saturated domain (2D).(Neumann, 2012)

Our results of gas saturation and molar fraction of dissolved CO_2 in water correlates qualitatively with the reference results despite the neglecting of compressibility.

- What is the compressibility role ?
- What is the EOS choice impact ?

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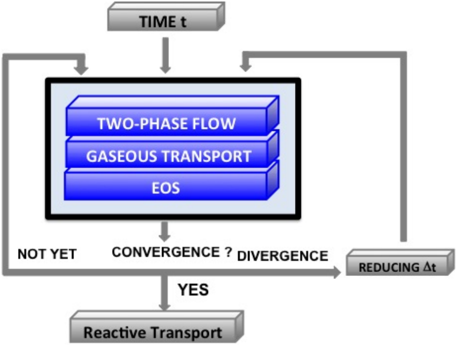
Compressible coupled 2-Phase Flow in HYTEC



Compressible coupled 2-Phase Flow in HYTEC

- Two-phase flow, $\alpha = \{l, g\}$

$$\frac{\partial \omega \rho_\alpha S_\alpha}{\partial t} + \mathrm{div}(\rho_\alpha \overrightarrow{u_\alpha}) + R_\alpha = 0$$
$$\overrightarrow{u_\alpha} = -\frac{k_{r\alpha}}{\mu_\alpha} K \left(\overrightarrow{\mathrm{grad}} p_\alpha - \rho_\alpha \overrightarrow{g} \right)$$

- Gas transport

$$\frac{\partial \omega S_g c_i^g}{\partial t} = \mathfrak{T}^g \left(c_i^g\right) + R_i^g \left(c_i^g\right)$$
$$\mathfrak{T}\left(c_i^g\right) = \mathrm{div}(D(S_g, D_g)\overrightarrow{\mathrm{grad}} c_i^g - c_i^g \overrightarrow{u_g})$$

- Equation of State

$$P = f(v, T, y_i)$$

Compressible coupled 2-Phase Flow in HYTEC

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- Equation of State

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Compressible coupled 2-Phase Flow in HYTEC

- Two-phase flow, $\alpha = \{g\}$

$$\frac{\partial \omega \rho_\alpha S_\alpha}{\partial t} - \mathrm{div}(\rho_\alpha \frac{k_{r\alpha}}{\mu_\alpha} K \left(\overrightarrow{\mathrm{grad}} p_\alpha - \rho_\alpha \overrightarrow{g}\right)) + R_\alpha = 0$$

- Gas transport

$$\frac{\partial \omega S_g c_i^g}{\partial t} = \mathrm{div}(D(S_g, D_g)\overrightarrow{\mathrm{grad}} c_i^g - c_i^g \overrightarrow{u_g}) + R_i^g \left(c_i^g\right)$$

- Equation of State

$$\rho_{g,mass} = \frac{\sum_{i=1}^{N} y_i M_i}{v}$$

$\rho_g(P)$ is continuous and strictly increasing. The gas density derivatives were added in the analytical Jacobian of two-phase flow.
The liquid density is constant during the current time step : it is taken from the previous time step.

Compressible coupled 2-Phase Flow in HYTEC

- Two-phase flow $\boldsymbol{F}(\boldsymbol{\zeta}) = 0$:

$$\frac{\rho_\alpha^{n+1,k} S_\alpha^{n+1,k+1} - \rho_\alpha^n S_\alpha^n}{\Delta t^{n+1,k+1}} = \mathfrak{F}\left(S_\alpha^{n+1,k+1}, p_\alpha^{n+1,k+1}\right)$$

- Gas transport

$$\frac{S_g^{n+1,k+1} c_i^{k+1} - S_g^n c_i^n}{\Delta t^{n+1,k+1}} = \sigma\, \mathfrak{T}\left(c_i^{k+1}\right) + (1-\sigma)\, \mathfrak{T}\left(c_i^n\right)$$

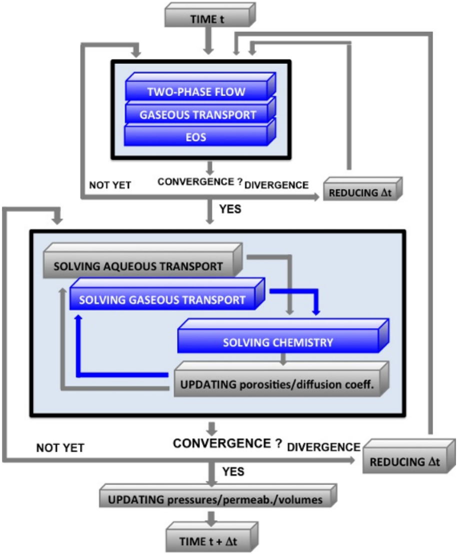
- Equation of State

$$\rho_g^{n+1,k+1} = \frac{\sum_{i=1}^N y_i^{n+1,k+1} M_i}{v^{n+1,k+1}}$$

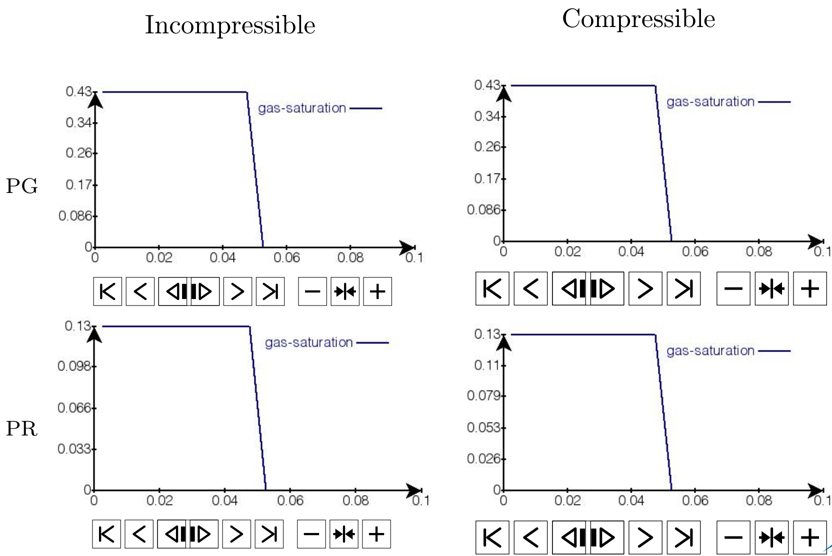
Stopping criterion :

$$\left(\|\boldsymbol{F}(\boldsymbol{\zeta}^{k+1})\|_2 \leq \varepsilon_{nl} \|\boldsymbol{F}(\boldsymbol{\zeta}^0)\|_2\right) \wedge$$
$$\left(|n_{gas}^{n+1,k+1} - n_{gas}^{n+1,k}| \leq \varepsilon_{gastr}\; n_{gas}^{n+1,k+1}\right) \wedge$$
$$(k+1 < k_{max})$$

Compressible coupled 2-Phase Flow in HYTEC



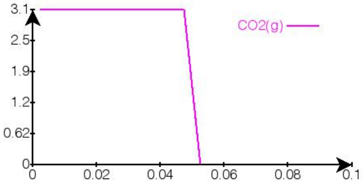
Test 1D. Gas Saturation

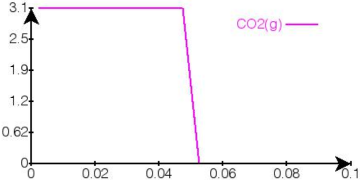


Test 1D. $CO_{2(g)}$, mol/l

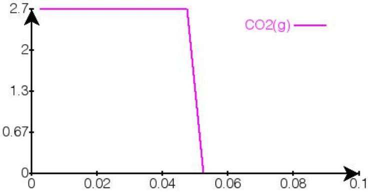
Incompressible | Compressible

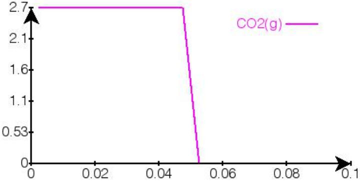
PG





PR





Conclusions and Perspectives

- Two-phase flow implementation in reactive transport software HYTEC.
- Preliminary tests of compressible two-phase flow with reactive transport.
- Improvement of coupling. Geochemical reactions.
- Prospective application :
  - Preferential H_2S leaching by active aquifer
    Workshop to be held from October 6 - 8, 2014 in Cadarache, South of France :
    Multiphase reactive transport modeling of a deep acid gas reservoir (benchmark proposal)
    http ://www-cadarache.cea.fr/gb/workshop.php
    contact person : irina.sin@mines-paristech.fr