

A Coats-Based Formulation for Multiphase Reactive Transport: Application to Hydrogen Storage in Porous Media

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- Extend the Coats formulation to multiphase reactive transport,
- Properly handle phase disappearance (especially the aqueous phase),
- Use a Globally Implicit Approach.

- 1 Reactive transport model
- 2 Phase appearance and disappearance
- 3 Numerical results

Notations (Morel's formalism)

- Primary species:

$$\mathcal{E}^{\text{pr}} = \{e_1^{\text{pr}}, \dots, e_M^{\text{pr}}\}.$$

- Secondary species:

$$\mathcal{E}^{\text{sec}} = \{e_1^{\text{sec}}, \dots, e_{N-M}^{\text{sec}}\},$$

such that each secondary species is associated to the chemical reaction:

$$e^{\text{sec}} \rightleftharpoons \sum_{e^{\text{pr}} \in \mathcal{E}^{\text{pr}}} E_{e^{\text{pr}}, e^{\text{sec}}} e^{\text{pr}},$$

where

$$E := [E_{e^{\text{pr}}, e}]_{e^{\text{pr}} \in \mathcal{E}^{\text{pr}}, e \in \mathcal{E}} \in \mathbb{R}^{\mathcal{E}^{\text{pr}} \times \mathcal{E}}.$$

- We set $\mathcal{E} := \mathcal{E}^{\text{pr}} \cup \mathcal{E}^{\text{sec}}$.

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- We set $\mathcal{E} := \mathcal{E}^{\text{pr}} \cup \mathcal{E}^{\text{sec}}$.
- To link a species $e \in \mathcal{E}$ to its phase $\beta \in \mathcal{P}$:

$$\alpha : e \in \mathcal{E} \mapsto \alpha(e) \in \mathcal{P}.$$

Total conservation equation

Total conservation

$$\sum_{e \in \mathcal{E}} E_{e^{\text{pr}}, e} \partial_t n_e + \sum_{e \in \mathcal{E}^f} E_{e^{\text{pr}}, e} \operatorname{div} \left(\zeta^{\alpha(e)} C_e u^{\alpha(e)} \right) = 0, \quad \forall e^{\text{pr}} \in \mathcal{E}^{\text{pr}},$$

where

- n_e [$\text{mol} \cdot \text{m}^{-3}$]: volumetric molar concentration of e , equals to

$$n_e = \phi \zeta^{\alpha(e)} S^{\alpha(e)} C_e, \quad \forall e \in \mathcal{E}^f,$$

- ϕ [–]: porosity,
- ζ^β [$\text{mol} \cdot \text{m}^{-3}$]: phase molar density,
- S^β [–]: phase saturation,
- C_e [–]: mole fraction of e in its phase,
- u^β [$\text{m} \cdot \text{s}^{-1}$]: follows the Darcy's law.

Chemical reactions

- Phase transition: Fugacity equality.
- Chemical equilibrium: Law of mass action,

$$Q := \frac{1}{a_{e^{\text{sec}}}} \prod_{e^{\text{pr}} \in \mathcal{E}^{\text{pr}}} (a_{e^{\text{pr}}})^{E_{e^{\text{pr}}, R}} = K_R.$$

- Kinetic reaction: Conservation equation with reaction rate T_e ,

$$\begin{aligned} \partial_t n_e + \text{div} \left(\zeta^{\alpha(e)} C_e u^{\alpha(e)} \right) &= T_e, \text{ if } e \text{ is a fluid kinetic species,} \\ \partial_t n_e &= T_e, \text{ if } e \text{ is a solid kinetic species.} \end{aligned}$$

Closure equations

- Total volume conservation:

$$\underbrace{\phi}_{\text{fluid}} + \underbrace{\phi^s + 1 - \phi_T}_{\text{solid}} = 1 \quad \Leftrightarrow \quad \phi + \phi^s = \phi_T,$$

where

- ϕ^s : volume fraction of reactive rock,
- $1 - \phi_T$: volume fraction of non-reactive rock.

- Closure relations:

$$\sum_{\beta \in \mathcal{P}^f} S^\beta = 1, \quad \sum_{e \in \alpha^{-1}(\{\beta\})} C_e = 1, \quad \forall \beta \in \mathcal{P}^f \quad \text{and} \quad \phi^s = \sum_{m \in \mathcal{P}^s} \frac{n_m}{\zeta^m}.$$

Summary

- $\#\mathcal{E} + \#\mathcal{P}^f + 2$ equations:
 - $\#\mathcal{E}^{\text{pr}}$: the conservation equations for total primary species,
 - $\#\mathcal{E}^{\text{sec}}$: one algebraic or differential equation for each equilibrium or kinetic chemical reaction, respectively,
 - $\#\mathcal{P}^f + 2$: closure equations,
- $\#\mathcal{E} + \#\mathcal{P}^f + 2$ natural variables (Coats formulation):
 - pressure P ,
 - saturations S^β , $\beta \in \mathcal{P}^f$,
 - solid porosity ϕ^s ,
 - molar fractions C_e , $e \in \mathcal{E}^f$,
 - molar concentrations n_e , $e \in \mathcal{E}^s$.

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Remark

Here, we assume that all phases are present!

- 1 Reactive transport model
- 2 Phase appearance and disappearance
- 3 Numerical results

Discretization

- Finite volume with TPFA and upwind scheme,

Discretized conservations of total primary species

for $e \in \mathcal{E}^{\text{pr}}$,

$$\sum_{e' \in \mathcal{E}} E_{e,e'} |K| \left(\chi_K(e') n_{e',K} - \chi_K^{n-1}(e') n_{e',K}^{n-1} \right) + \Delta t^n \sum_{e' \in \mathcal{E}^{\text{f}}} \sum_{\sigma=K | L \in \mathcal{F}_K \cap \mathcal{F}_h} \chi_{K_\sigma}^{\alpha(e')}(e') E_{e,e'} \left(\zeta^{\alpha(e')} C_{e'} \eta^{\alpha(e')} \right)_{K_\sigma^{\alpha(e')}} V_{KL}^{\alpha(e')} = 0,$$

where

- $\mathcal{Q}_K = (\mathcal{Q}_K^{\text{f}}, \mathcal{Q}_K^{\text{s}})$: set of present fluid/solid phases in K ,
- $\chi_K(e) := 1_{\mathcal{Q}_K}(\alpha(e))$ (analog for $\chi_K^{n-1}(e)$).

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Problem

Singularity issue if a primary species disappears.

Discretization

- Additional concentration unknowns chosen based on the rank deficiency of the formula matrix restricted to the present species:

$$\tilde{n}_{e,K}, \quad e \in \tilde{\mathcal{E}}_{Q_K},$$

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for $e \in \mathcal{E}^{\text{pr}}$,

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Remarks

- Regularize the Jacobian matrix,
- Track incoming flux from surrounding cells (phases reappearance).

Phase appearance and disappearance

Phase removal

- Fluid phase β disappears if $S^\beta < 0$.
- Mineral phase m disappears if $n_m < 0$.

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Phase appearance with liquid phase

- A mineral phase appears when its solubility product exceeds equilibrium.
- A gas phase appears if

$$\tilde{n}_e > 0$$

for any gas species e in $\tilde{\mathcal{E}}_{Q_K}$, or if

$$\sum_e \tilde{C}_e > 1.$$

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Without liquid phase

A multiphase flash calculation is performed at fixed total composition.

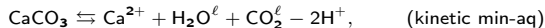
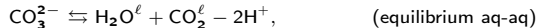
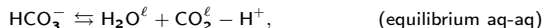
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Settings

- Primary species (4):

$$\mathcal{E}^{\text{pr}} = \{\text{H}_2\text{O}^\ell, \text{CO}_2^\ell, \text{H}^+, \text{Ca}^{2+}\},$$

- Reactions (6):



- Phases: $\mathcal{P} = \{\ell, g, m_{\text{CaCO}_3}\},$

Additional unknowns (CO_2 test case)

$$E := \begin{pmatrix} \text{H}_2\text{O}^\ell & \text{CO}_2^\ell & \text{H}^+ & \text{Ca}^{2+} & \text{HCO}_3^- & \text{OH}^- & \text{CO}_3^{2-} & \text{H}_2\text{O}^g & \text{CO}_2^g & \text{CaCO}_3 \\ \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} & \begin{pmatrix} 1 & 1 & 1 \\ 1 & 0 & 1 \\ -1 & -1 & -2 \\ 0 & 0 & 0 \end{pmatrix} & \begin{pmatrix} 1 & 0 & -2 \\ 1 & 1 & 1 \\ -2 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix} \end{pmatrix} \begin{pmatrix} \text{H}_2\text{O}^\ell \\ \text{CO}_2^\ell \\ \text{H}^+ \\ \text{Ca}^{2+} \end{pmatrix}.$$

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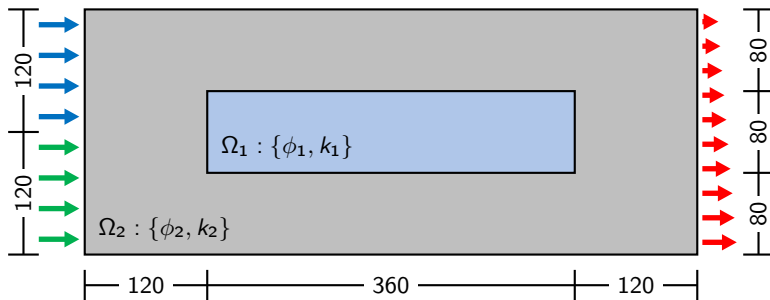
$$E_{Q_K} = \left(\begin{array}{cc} \text{H}_2\text{O}^g & \text{CO}_2^g \\ 1 & 0 \\ 0 & 1 \\ 0 & 0 \\ 0 & 0 \end{array} \right), \text{ if } Q_K = \{g\}.$$

$$E_{Q_K} = \left(\begin{array}{ccc} \text{H}_2\text{O}^g & \text{CO}_2^g & \text{CaCO}_3 \\ 1 & 0 & 1 \\ 0 & 1 & 1 \\ 0 & 0 & -2 \\ 0 & 0 & 1 \end{array} \right), \text{ if } Q_K = \{g, m_{\text{CaCO}_3}\}$$

- Rank: 2,
- Two additional unknowns: $\tilde{n}_{\text{H}^+}$ and $\tilde{n}_{\text{Ca}^{2+}}$.

- Rank: 3,
- One additional unknown: $\tilde{n}_{\text{H}^+}$ (or $\tilde{n}_{\text{Ca}^{2+}}$).

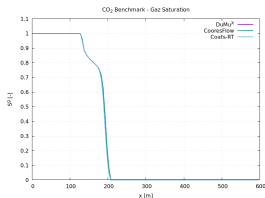
Settings



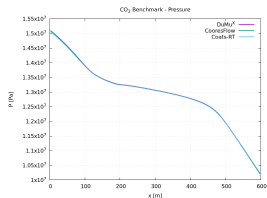
- Gas stream (pure CO_2^g): Q_{gas} [m^3/day]
- Water stream (pure H_2O^ℓ): Q_{wat} [m^3/day]
- Outflow (hydrostatic pressure): p_{out} [bar]

Results

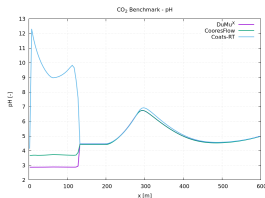
Code team	TS (failed)	NI	F (failed)	CPU	Architecture
DuMu ^X	17571 (2937)	3.45	-	66124	Intel i7-8565U @1.8 GHz
CooresFlow	2008 (0)	4.1	-	10224	Intel Xeon E5-1620 v3 @3.5 GHz
Coats-RT	2032 (8)	5.2	206939 (0)	6361	Intel Core Ultra 7 255H @2.0 GHz



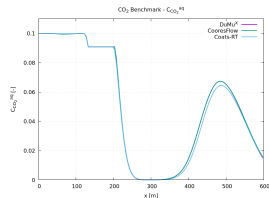
(d) Gas Saturation



(e) Pressure



(f) pH



(g) $C_{\text{CO}_2^{\text{aq}}}$

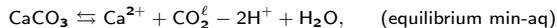
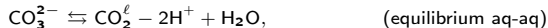
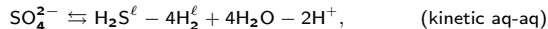
Figure: Benchmark – DuMu^X, CooresFlow and Coats-RT.

Settings

- Primary species (7):

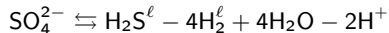
$$\mathcal{E}^{\text{Pr}} := \{\text{H}_2\text{S}^\ell, \text{H}_2^\ell, \text{CO}_2^\ell, \text{H}_2\text{O}, \text{H}^+, \text{Ca}^{2+}, \text{Na}^+\}.$$

- Reactions (9):



- Phases: $\mathcal{P} = \{\ell, g, m_{\text{CaCO}_3}\}.$

Settings



- Monod-type law: (bacterial activity)

$$T_{\text{SO}_4^{2-}} = -v_{\max} \frac{10^{-3}\zeta^\ell C_{\text{SO}_4^{2-}}}{10^{-3}\zeta^\ell C_{\text{SO}_4^{2-}} + K_{\text{SO}_4^{2-}}} \frac{10^{-3}\zeta^\ell C_{\text{H}_2^\ell}}{10^{-3}\zeta^\ell C_{\text{H}_2^\ell} + K_{\text{H}_2^\ell}},$$

with

- $v_{\max} = 1.45 \times 10^{-5} \text{ mol} \cdot \text{L}^{-1} \cdot \text{year}^{-1}$,
- $K_{\text{SO}_4^{2-}} = 10^{-4} \text{ mol} \cdot \text{L}^{-1}$, and $K_{\text{H}_2^\ell} = \varepsilon \text{ mol} \cdot \text{L}^{-1}$.

Additional unknowns (H_2 test case)

$$E := \left(\begin{array}{cccccc|cccccccc} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & -4 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 4 & 0 & 1 & 1 & 1 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & -2 & -1 & -1 & -1 & -2 & 0 & 0 & 0 & -2 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{array} \right).$$

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► If $\mathcal{Q}_K = \{g\}$:

$$E_{\mathcal{Q}_K} = \begin{pmatrix} \text{H}_2\text{S}^g & \text{H}_2^g & \text{CO}_2^g \\ 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

- Rank: 3,
- Four additional unknowns: $\tilde{n}_{\text{H}_2\text{O}}$, $\tilde{n}_{\text{H}^+}$, $\tilde{n}_{\text{Ca}^{2+}}$ and $\tilde{n}_{\text{Na}^+}$.

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► If $\mathcal{Q}_K = \{g, m_{\text{CaCO}_3}\}$:

$$E_{\mathcal{Q}_K} = \begin{pmatrix} \text{H}_2\text{S}^g & \text{H}_2^g & \text{CO}_2^g & \text{CaCO}_3 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & -2 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \end{pmatrix}.$$

- Rank: 4,
- Three additional unknowns: for example $\tilde{n}_{\text{H}_2\text{O}}$, $\tilde{n}_{\text{H}^+}$ and $\tilde{n}_{\text{Na}^+}$.

Settings

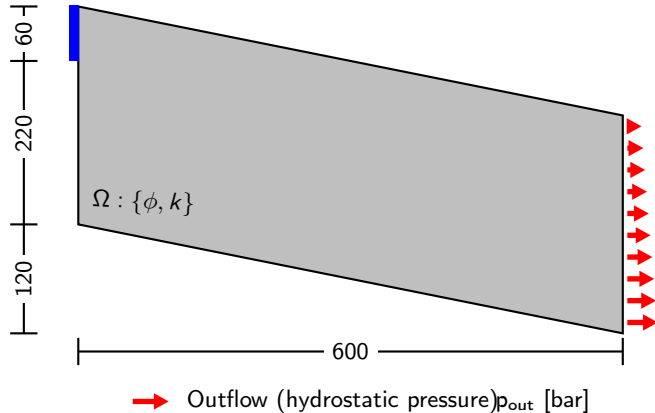


Figure: Configuration of the H_2 injection test case.

Simplified vertical well model

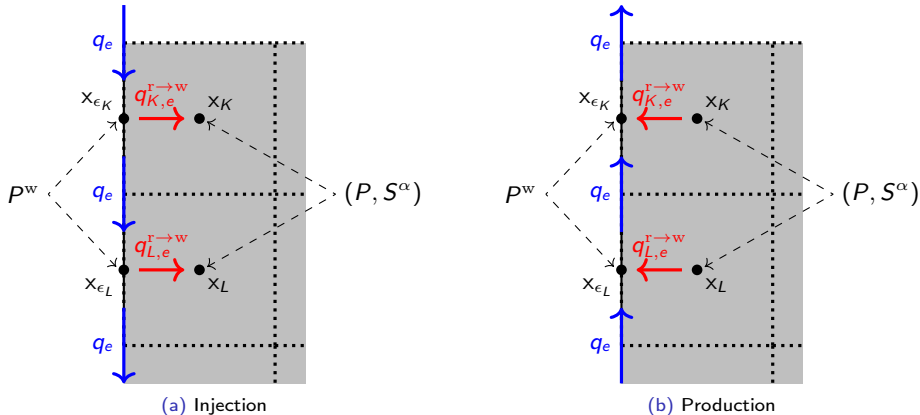


Figure: Discretization of the well on a cartesian mesh.

Simplified vertical well model

- Injection:

$$q_{K,e}^{r \rightarrow w} = \begin{cases} \zeta^g(P_K^w) \eta^g(1) k \text{ WI} \min(0, P_K - P_K^w) & \text{if } e = \text{H}_2^g, \\ 0 & \text{otherwise,} \end{cases} \leq 0,$$

- Production:

$$q_{K,e}^{r \rightarrow w} := \zeta^{\alpha(e)}(P_K) \eta^{\alpha(e)}(S_K^{\alpha(e)}) k \text{ WI} \max(0, P_K - P_K^w) \geq 0,$$

with

- k is the permeability [m^2] assuming a homogeneous and isotropic medium (i.e. $\mathbb{K} = k \text{ Id}$),
- WI is the well index [m].

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Well equation

$$\left(\sum_{K \in \mathcal{M}^w} \sum_{e \in \mathcal{E}^{\text{pr}} \cap \mathcal{E}^f} \sum_{e \in \mathcal{E}^f} E_{e^{\text{pr}},e} q_{K,e}^{r \rightarrow w} - \bar{Q} \right) (P_{\text{bh}}^w - \bar{P}) = 0.$$

where $\mathcal{M}^w$ is the set of reservoir cells connected to the well and $P_K^w = P_{\text{bh}}^w + \Delta P_K^w$.

Simplified vertical well model – Well Index

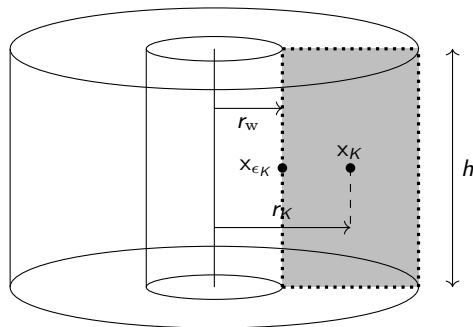
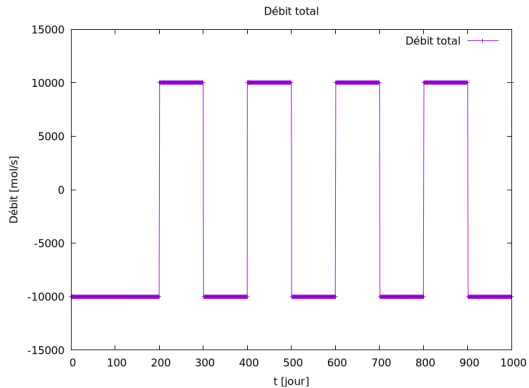


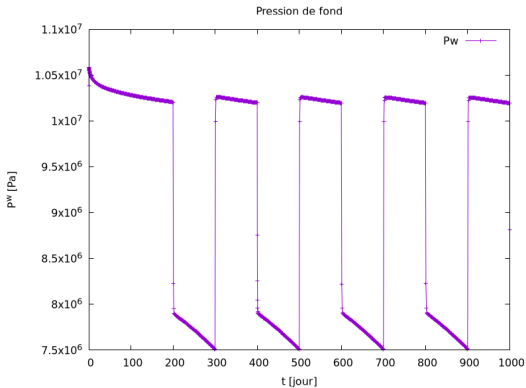
Figure: Discretization in radial geometry.

$$\text{WI} = \frac{2\pi h}{\ln(r_K/r_w)}$$

Results

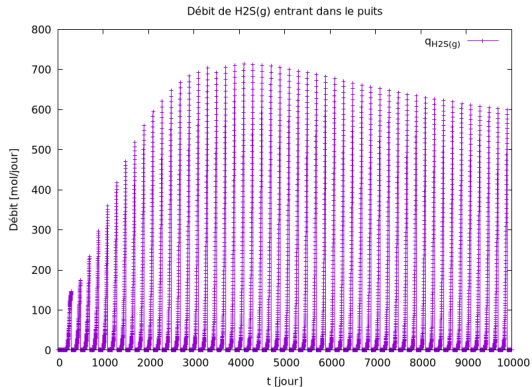


(a) Total molar flow rate

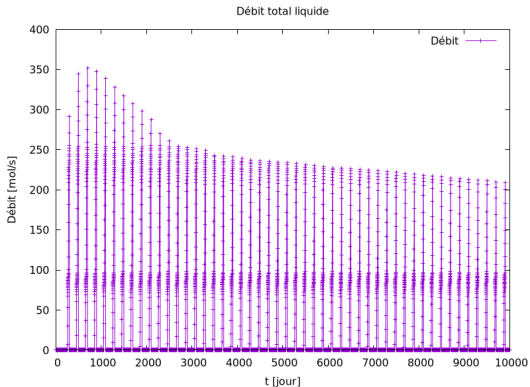


(b) P_{bh}^w

Results

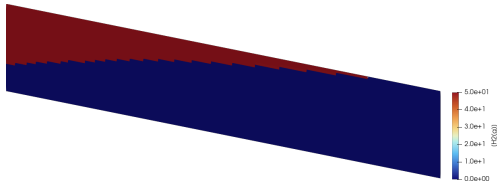


(c) H_2S^g

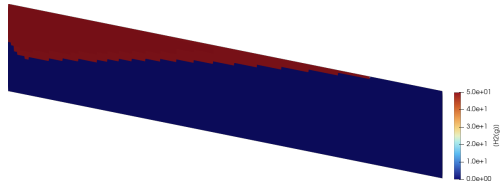


(d) Total molar flow rate

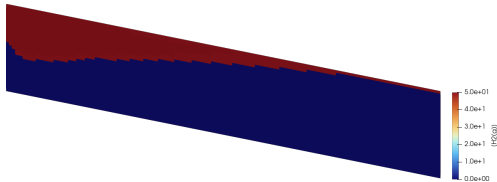
Results – H_2^g



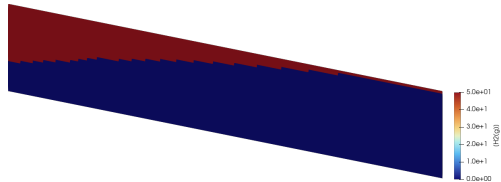
(e) $t = 200$ days



(f) $t = 300$ days

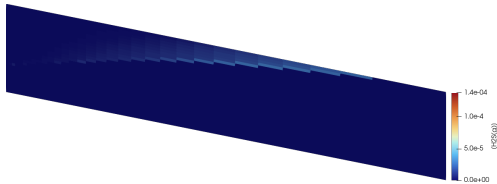


(g) $t = 900$ days

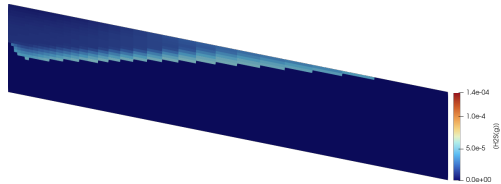


(h) $t = 1000$ days

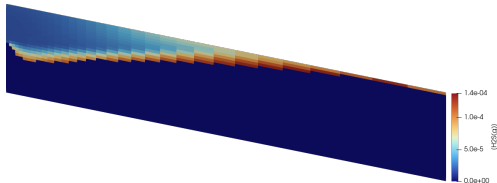
Results – H_2S^g



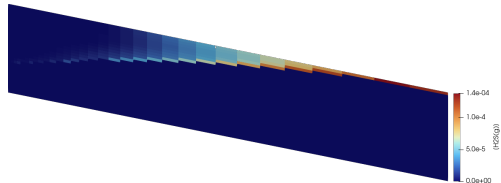
(i) $t = 200$ days



(j) $t = 300$ days

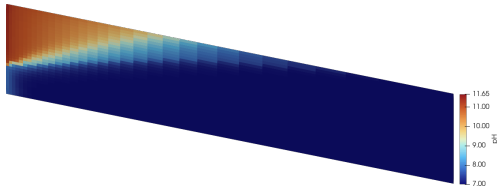


(k) $t = 900$ days

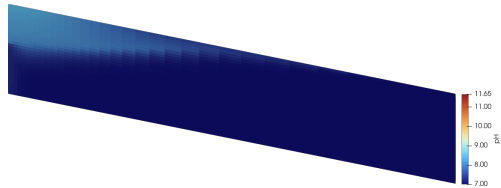


(l) $t = 1000$ days

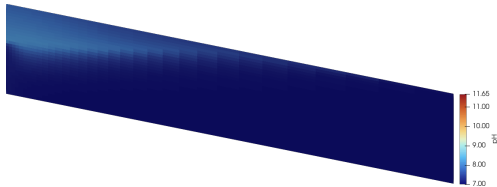
Results – pH



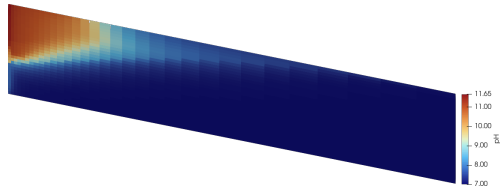
(m) $t = 200$ days



(n) $t = 300$ days



(o) $t = 900$ days



(p) $t = 1000$ days

Conclusion and perspectives

Conclusion

- Fully implicit multiphase reactive transport model based on Morel's and Coats' formulations.
- Robust handling of phase appearance/disappearance, including the aqueous phase.
- Validate the method and the implementation on the CO_2 benchmark.
- Application to a 2D axisymmetric hydrogen storage with injection/production cycles.

Future work

- More realistic testcase (pH buffering reactions, methanation, gaseous H_2O , ...).

Thank you for your attention!