

EAGE



European Conference on the Mathematics of Geological Reservoirs

8-11 SEPTEMBER 2026 | PORTO, PORTUGAL

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Abstract No. 78

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

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Objectives

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

Reactive transport model

Phase appearance and disappearance

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

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

where

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

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

- 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.

- 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 ,

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

Closure equations

- Total volume conservation:

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

where

- ▶ ϕ^{s} : volume fraction of reactive rock,
- ▶ $1 - \phi_{\text{T}}$: volume fraction of non-reactive rock.

- Closure relations:

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

- $\#\mathcal{E} + \#\mathcal{P}^f + 2$ 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!

Reactive transport model

Phase appearance and disappearance

Numerical results

- Finite volume with TPFA and upwind scheme,

Discretized conservations of total primary species

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

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

where

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

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

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

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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.

Reactive transport model

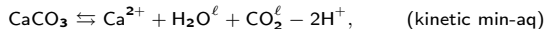
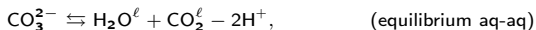
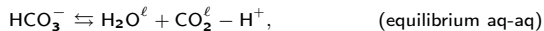
Phase appearance and disappearance

Numerical results

- 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 (CO₂ test case)

$$E := \left(\begin{array}{cccc|cccccc} \text{H}_2\text{O}^\ell & \text{CO}_2^\ell & \text{H}^+ & \text{Ca}^{2+} & \text{HCO}_3^- & \text{OH}^- & \text{CO}_3^{2-} & \text{H}_2\text{O}^g & \text{CO}_2^g & \text{CaCO}_3 \\ 1 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & 0 & 1 \\ 0 & 1 & 0 & 0 & 1 & 0 & 1 & 0 & 1 & 1 \\ 0 & 0 & 1 & 0 & -1 & -1 & -2 & 0 & 0 & -2 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 \end{array} \right) \begin{array}{l} \text{H}_2\text{O}^\ell \\ \text{CO}_2^\ell \\ \text{H}^+ \\ \text{Ca}^{2+} \end{array}.$$

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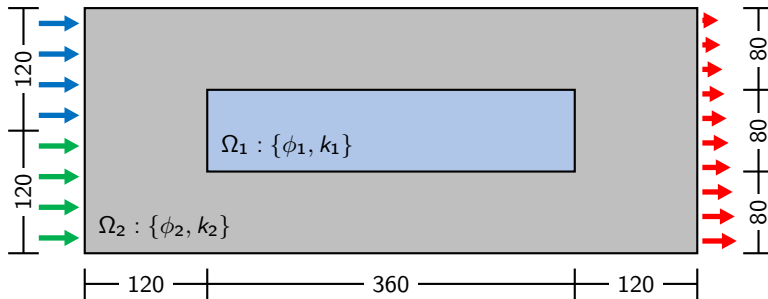
$$E_{Q_K} = \left(\begin{array}{cc} \text{H}_2\text{O}^g & \text{CO}_2^g \\ 1 & 0 \\ 0 & 1 \\ 0 & 0 \\ 0 & 0 \end{array} \right), \text{ if } Q_K = \{g\}.$$

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

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

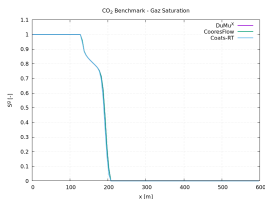
- Rank: 3,
- One additional unknown: $\tilde{n}_{\text{H}^+}$ (or $\tilde{n}_{\text{Ca}^{2+}}$).

Settings

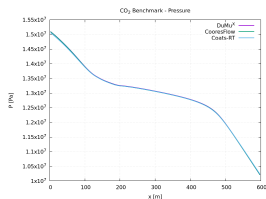


- Gas stream (pure CO_2^g): Q_{gas} [m^3/day]
- Water stream (pure H_2O^ℓ): Q_{wat} [m^3/day]
- Outflow (hydrostatic pressure): p_{out} [bar]

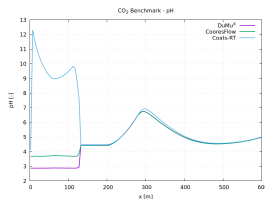
Code team	TS (failed)	NI	LI / NI	F (failed)	CPU	Architecture
DuMu ^X	17571 (2937)	3.45	8.37	-	66124	Intel i7-8565U @1.8 GHz
CooresFlow	2008 (0)	4.1	not available	-	10224	Intel Xeon E5-1620 v3 @3.5 GHz
Coats-RT	2032 (8)	5.2	11.76	206939 (0)	6361	Intel Core Ultra 7 255H @2.0 GHz



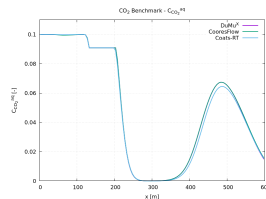
(d) Gas Saturation



(e) Pressure



(f) pH

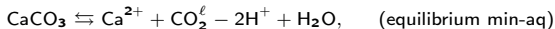
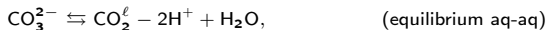
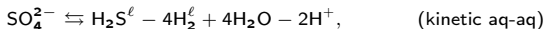
(g) C_{CO₂^g}Figure: Benchmark – DuMu^X, CooresFlow and Coats-RT.

Settings

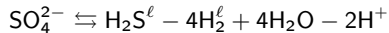
- Primary species (7):

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

- Reactions (9):



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



- 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 (H₂ test case)

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

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► If $\mathcal{Q}_K = \{g\}$:

$$E_{\mathcal{Q}_K} = \begin{array}{c} \text{H}_2\text{S}^g \quad \text{H}_2^g \quad \text{CO}_2^g \\ \left(\begin{array}{ccc} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{array} \right) \end{array}.$$

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

Additional unknowns (H_2 test case)

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

► 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

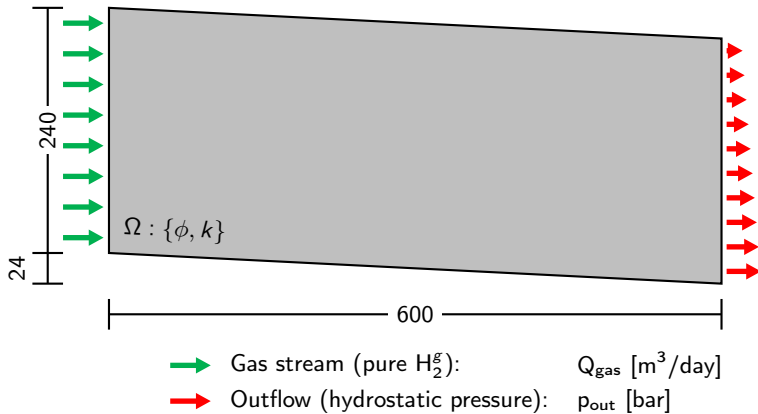
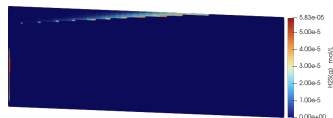
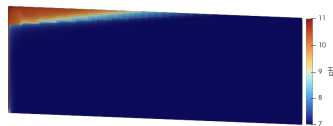


Figure: Radial geometry.

Results

(a) H_2^g at $t = 500$ days(b) H_2^g at $t = 1000$ days(c) H_2S^g at $t = 500$ days(d) H_2S^g at $t = 1000$ days(e) pH at $t = 500$ days(f) pH at $t = 1000$ days

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 CO₂ benchmark.
- Application to a 2D axisymmetric hydrogen injection scenario.

Future work

- Clay-fluid reactions for pH buffering.
- Injection and production well models.

Thank you for your attention!

Globally Implicit Approach

- At each time step n , the nonlinear system is solved using Newton's method.
- Adaptive time stepping: If Newton converges,

$$\Delta t^{n+1} = \min\{1.1 \Delta t^n, \Delta t_{\max}\}.$$

If Newton fails, the time step is halved and recomputed.

- At each Newton iteration:
 - ▶ assembly of the Jacobian and residual,
 - ▶ relaxed Newton update,
 - ▶ weighted ℓ^∞ norm residual based on pressure, saturations, fluid compositions and mineral concentrations.

- Convergence criteria:

$$\|R\|_\infty < 10^{-7} \quad \text{or} \quad \|\delta U\|_\infty < 10^{-10}.$$

- Linear systems are solved using CPR-AMG. Convergence is reached when

$$\frac{\|r_k\|_2}{\|r_0\|_2} < 10^{-7}.$$