Comparison of numerical schemes for multiphase reactive transport

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Outline

I. Introduction
   - Motivation
   - References
   - Problem description

II. Formulation and Active Set Algorithm

III. Splitting Algorithm

IV. Results

V. Conclusion and Future Work
1. Motivation

- Applications in Geosciences:
  - CO2 Sequestration
  - Gas Production and Storage
  - EOR
  - Mineral Diagenesis

- Other Applications:
  - Batteries
  - Biological processes
I. Problem Description

- Multi-Phase Multi-Species System
I. Problem Description

- Advection in Porous media

\[ \frac{\partial n_{j}^{\alpha}}{\partial t} + \text{div}(c_{j}^{\alpha} \vec{v}_{\alpha}) + R_{j}^{\alpha} = 0 \]

\[ n_{j}^{\alpha} = \phi \times S^{\alpha} \times \frac{\rho^{\alpha}}{M^{\alpha}} \times x_{j}^{\alpha} \]

\[ c_{j}^{\alpha} = \frac{\rho^{\alpha}}{M^{\alpha}} \times x_{j}^{\alpha} \]

\[ \vec{v}_{\alpha} = -\frac{k_{r}}{\mu^{\alpha}} \times K \times (\nabla P_{\alpha} + \rho_{\alpha} g \nabla z) \]
I. Problem Description

- Equilibrium chemical reactions
  - For each reaction \( r \)
    \[
    \Delta_r G = \sum_{j=1}^{n_s} s_{jr} \mu_j = 0
    \]

- Closure Equations

- Equilibrium reaction rates are unknown
  - Rates elimination using chemical analysis
I. Problem Description

- **Example System**
  - Water (H₂O, OH⁻, H⁺, HCO₃⁻, Ca⁺⁺), Gas (CO₂⁰), Calcite (CaCO₃ˢ)
    - H₂O = H⁺ + OH⁻
    - CO₂⁰ + H₂O = HCO₃⁻ + H⁺
    - HCO₃⁻ + Ca⁺⁺ = CaCO₃ˢ + H⁺

- **Formula matrix A**

<table>
<thead>
<tr>
<th></th>
<th>H₂O</th>
<th>H⁺</th>
<th>HCO₃⁻</th>
<th>Ca⁺⁺</th>
<th>OH⁻</th>
<th>CO₂⁰</th>
<th>CaCO₃ˢ</th>
</tr>
</thead>
<tbody>
<tr>
<td>N_{H₂O}</td>
<td>1</td>
<td></td>
<td></td>
<td></td>
<td>1</td>
<td>-1</td>
<td></td>
</tr>
<tr>
<td>N_{H⁺}</td>
<td></td>
<td>1</td>
<td></td>
<td></td>
<td>-1</td>
<td>1</td>
<td>-1</td>
</tr>
<tr>
<td>N_{HCO₃⁻}</td>
<td></td>
<td></td>
<td>1</td>
<td></td>
<td></td>
<td>1</td>
<td></td>
</tr>
<tr>
<td>N_{Ca⁺⁺}</td>
<td></td>
<td></td>
<td></td>
<td>1</td>
<td></td>
<td>1</td>
<td>1</td>
</tr>
</tbody>
</table>

- **13 equations (4 mass balance equations, 6 closure equations, 3 chemical equilibrium equations)**

- **13 variables (P, φᶠ, φˢ, Sₜ, Sₜ, Sₛ, x_{H₂O->CaCO₃ˢ})**
II. Formulation and Active Set Algorithm

- **Discretization**
  - Global Implicit Approach (Implicit Euler)
  - Two-points finite volume scheme

- **Issue with phase appearance and disappearance**
  - Complementarity conditions
  - Active Set algorithm vs Semi-smooth Newton methods

- **New context variable I**
  - \( I_k = \text{context of cell } k \)
  - Equations and variables depend on \( I_k \)
  - Split active and non-active species, components and equations
II. Formulation and Active Set Algorithm

- **Example continued**
  - $I_k = \{\text{Gas, Calcite}\}$

- 9 equations (4 mass balance equations, 5 closure equations, 0 chemical equilibrium equations) for cell $k$

- 9 variables ($P, \phi_f, \phi_s, S_g, S_s, x_{CO2g}, x_{CaCO3s}, N_{H2O}^l, N_{H+}^l$) for cell $k$
II. Formulation and Active Set Algorithm

- **Global non linear equation solver**
  - Each active variable is updated at the end of each Newton iteration
  - Context variable also needs to be updated
    - Negative saturation $\rightarrow$ phase disappearance
    - Equilibrium flash $\rightarrow$ phase appearance

- **Equilibrium flash can be any 0D chemistry solver**
  - LMA / GEM formulation
  - External or Internal library
III. Splitting Algorithm

- Splitting occurs at different stages

Diagram:

- Flow
- Reactive Transport
- Porosity update
- Transport
- Flash

Symbols:
- \( t_n \)
- \( t_{n+1} \)
- \( P, S_{\alpha} \)
- \( \phi \)
- \( n_j^a \)
IV. Results – Active Set

SHPCO2 case study
IV. Results – Active Set
IV. Results – Active Set
IV. Results – Active Set
IV. Results – Comparison

- SES Benchmark

Irina Sin and Jerome Corvisier, Ecole des Mines de Paris, Geosciences research center
IV. Results – Comparison

- Simple benchmark

```
Pressure

2.95e+07  3e+7  3.1e+7  3.2e+7

2.95e+07  3.24e+07

t = 3.1536e12 s = 100 000 ans
```
IV. Results – Comparison

\[ T = 100\,000\ \text{years} \]

- Active Set
- Splitting (Non iterative)
- Splitting (Iterative)
IV. Conclusion and Future Work

- Active Set algorithm to model multi-phase multi-species flow in porous media
- Comparison with splitting approach
- Future work involves
  - Non-Linear solver efficiency
  - Flash solver improvement
  - Semi-smooth Newton approach
  - Extension to kinetics and diffusion fluxes
Thank you