Reactive Transport Modeling By Using Eulerian-Lagrangian Methods Based on Mixing

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1. MOTIVATION

Reactive transport is involved in many natural phenomena such as degradation of pollutants, precipitation-dissolution processes of minerals, etc. The complexity of these phenomena and the difficulty of finding a single numerical method valid in any case make those modelling problems a difficult task to deal with. They often cause some additional fictitious dispersion so-called numerical dispersion, which is a serious problem especially in cases where equilibrium reactions are dominant, since reaction rate is proportional to the mixing De Simoni et al. 2005.

2. OBJECTIVE

Methodology to model Reactive transport that:
- Good characterization of mixing
- Performance in equilibrium reaction (controlled by mixing rate)
- Minimize numerical dispersion

3. METHOD

Decouple dispersion (spreading) from diffusion (mix)
\( \frac{D}{V} \cdot \frac{DC}{dt} \)
Decrease of dispersion coefficient
Advection domination problem
\( q \cdot \frac{V C}{dt} \)
Eulerian–Lagrangian method
\( \frac{DC}{dt} (x,t) = \frac{dc}{dt} + \frac{q}{V} \cdot \frac{C}{dt} = \frac{D}{V} \cdot \frac{dc}{dx} + f + rC \)

Mix
- Use of mass mixing fraction \( A \) to define transport.
- Here we express it explicitly

Advection
- Streamline oriented mesh
- Avoid numerical dispersion because no A has been defined for advection

Chemistry
- Decoupled from transport by using conservative components at different ways (Saaltink et al. 2003)
- Use of CHEPROO library (Bea et al. 2003)
- From transport code, only a water composition and \( A \) are defined to solve reactive transport

4. RESULTS

Instantaneous pulse injection
- Problem with analytical solution
- Precise performance without sharply initial fronts

Numerical solution
- Analytical solution

CAL
- Test example: dissolution of calcite by saturated infiltrating water
- Comparison with DSA method
- No numerical dispersion occurs in mixing method
- Decreasing CPU time

Two end members injection
- Problem with analytical solution
- Precise results along whole axis

WAD
- Test example: flashing of saline water by fresh water (Saaltink and Poole 1992)
- Comparison with DSA method
- Numerical dispersion occurs due adsorption
- CPU time decreased markedly from DSA

5. CONCLUSIONS

- This work presents a new reactive transport method based on mixing, which decouples chemistry from transport.
- It has been verified that method is refined when no steep fronts exist
- The proposed method allows to simulate with free of numerical dispersion when no adsorption occurs
- It can be stated that the CPU time cost is reduced in comparison with DSA method, specially in problems with large number of nodes.

References

Acknowledgements
- J. Soler wishes to acknowledge the financial support received from the AGAUR (Government of Catalonia, Spain) through the “Grant for universities and research centers for the recruitment of new research personnel (IJCUB 2013).”
- This work has been funded by the Global CCS Institute and by the European Community’s Seventh Framework Programme FP7/2007-2013 through the TIGOT and the FANAZA projects.