Comparison of PFLOTRAN and TOUGHREACT numerical codes for reactive transport modelling of CO_2 storage in saline aquifers

B. CANTUCCI[1]* P. ORSINI[2] AND F. QUATTROCCHI[1]

[1]Istituto Nazionale di Geofisica e Vulcanologia, Via di Vigna Murata 605, 00143 Rome, Italy (*correspondence: barbara.cantucci@ingv.it)

[2]BLOSint Ltd, University of Nottingham Innovation Park, Triumph road, NG7 2TU (paolo.orsini@blosint.com)

CO_2 geological storage in deep saline aquifers needs specific requirements in terms of safe storage and enduring containment of injected gas.

In order to understand the behaviour of CO_2 and predict the effect of geochemical reactions on trapping meachanisms and porosity/peremability variations, numerical models are an important tool.

Due to the large time and length scales involved, realistic numerical solutions, including thermal, hydrologeological and geochemical effects, are computationally demanding and the use of parallel software is necessary.

In this work a large scale model of an Italian reservoir, potentially suitable for CO_2 storage, is used as case study to compare two reactive transport codes, TOUGHREACT [1] and PFLOTRAN [2]. Pflotran is an open-source, 3D reservoir simulator, for sub-surface multiphase, multicomponent reactive flows with parallel capabilities.

The simulation model consists of an offshore structure with an area of more than 100 km^2 and a vertical development of 3 km, hosting a thick carbonatic reservoir. Two simulations were performed at different scales, considering advective and diffusive transport of the considered species at non-isothermal conditions and mineral reactions kinetically controlled. The feedback between flow and geochemical reactions, implemented in PFLOTRAN, has been customised in order to comply with the model implemented in TOUGHREACT.

At the time of writing the Authours are finalising the comparison between PFLOTRAN and TOUGHREACT solutions. However, from the preliminary results, some divergences found are likely to be due to the different EOS used to compute the dissolution of supercritical CO_2 in brine. Grid sensivity analysis and boundary condition effects are also being investigated as part of the software comparison.

[1] Xu *et al*. (2006) Computer & Geosciences **32**, 145–165. [2] Hammond *et al*. (2012) Groundwater Reactive Transport Models **5**, 142-160.

Research on particles carried by ascending gas flow of earthquake ruptures

JIANJIN CAO [12]*, SONGYING LUO[1], PEIXIN LAI[1], ZHENGYANG WANG[1], YIPENG LIAO[1] AND JIE YI[1]

[1]Department of Earth Science, Sun Yat-sen University, Guangzhou, China

[2] Guangdong Key Laboratory of Geological Process and Mineral Resources Exploration, Guangzhou, China

* correspondence: (eescjj@mail.sysu.edu.cn)

Last century, Kristiansson and Malmqvist put forward that element contents of material carried by the the naturally occurring ascending gas flow from earth interior were analyzed and the data can be used in exploration of metal deposits. [1] Many researchers studied the application effect in metal deposits of the method. [2] We proposed and studied that the concealed metal deposits were detected using the type, size, shape, structure, chemical composition of the particles carried by the ascending gas flow. [3]-[5] In the last few years, It's the first time that we proposed that release of a large amount of particles in gases from Earth's interior were caused by earthquake and the characteristics of the particles can be used in earthquake prediction.

We studied that the type, size, shape, structure, chemical composition of particles as well as gathering characteristic among the particles, which were carried by the ascending gas of ruptures generated by the “5.12” great wenchuan earthquake, using the individual particle analysis technology of a transmission electron microscopy. Similarities and differences in the particle characteristics of ascending gas between the ruptures generated by the “5.12” great wenchuan earthquake and the fault without earthquake occurrence were compared. Abnormal particles, which are rich in metals such as Pb, Hg, Cu, Os, were found in the ascending gas of ruptures generated by the “5.12” great wenchuan earthquake.

The particles offered the new data that derives from the depth for study on causes of earthquake. This research provided a new method for earthquake prediction. It can enrich theory of nanogeoscience.

The authors acknowledge the support of the National Natural Science Foundations of China (Grant Nos. 41072263, and 41030425) and the National High-Tech Research and Development Program of China (Grant No. 2008AA06Z101).

[1] Kristiansson *et al*. (1982) *Geophysics*. **47**, 1444–1452. [2]Wang *et al*.(1999) *Journal of Geochemical Exploration* **66**, 85-97. [3] Cao *et al*. (2009) *Journal of Geochemical Exploration* **101**, 247–253. [4] Cao *et al*. (2010) *Science China Earth Sciences* **53**, 1647–1654. [5] Cao. (2011) *Geochemical Journal* **45**, e9 ~e13.

DOI: 10.1180/minmag.2013.077.5.3