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Feasibility and validation procedure of a geochemical modeling applied to CO₂ storage: a new approach

Cantucci B. (1,2), Montegrossi G. (3), Tassi F. (3), , Vaselli O. (2,3), Buccianti A.(2), Quattrocchi F. (1)

(1) INGV, Rome 1 Section, Via di Vigna Murata 605, Rome, 00143, Italy; (2) Earth Science Dept., University of Florence, Via La Pira 4, Florence, 50121, Italy; (3) CNR - IGG, Via La Pira 4, Florence, 50121, Italy; (cantuccib@alice.it)

 CO_2 geological storage is one of the most promising technologies for reducing atmospheric emissions of greenhouse gas. The results obtained by a new approach applied to a CO_2 storage geochemical model at the Weyburn (Saskatchewan, Canada) test site, where since September 2000 5000 t/day of supercritical CO_2 are injected, are presented and discussed. The Weyburn oil-pull is recovered from the Midale Beds (at the depth of 1300-1500 m), consisting of Mississippian shallow marine carbonateevaporites, that is classically subdivided into two units: i) the dolomitic "Marly" and ii) the underlying calcitic "Vuggy", sealed by an anhydrite cap-rock.

Assumptions and gap-acceptance are commonly made to reconstruct the reservoir conditions (pressure, pH, chemistry, and mineral assemblage), although most geochemical parameters of deep fluids are to be computed by *a posteriori* procedure due to the sampling collection at the well-head, i.e. using depressurised aliquots. On the basis of the available data at Weyburn, such as: *a*) bulk mineralogy of the Marly and Vuggy reservoirs; *b*) mean gas-cap composition at the well-heads and *c*) selected preand post-CO₂ injection water samples, we have rebuilt the in-situ reservoir chemical composition and the kinetic evolution after CO₂ injection. The geochemical modelling has been performed by using the code PRHEEQC (V2.11) software package; the in-situ reservoir composition was calculated by the chemical equilibrium among the various phases at reservoir temperature (62 °C) and pressure (150 bars) via thermodynamic corrections to the code default database. Furthermore, the "primitive" chemical composition of the pre-injection Marly and Vuggy liquid phase was derived by assuming the equilibrium conditions for the mineral assemblage with respect to a Na-Cl

(Cl/Na=1.2) water. A comparison between the chemical composition of the "primitive brine" and that measured before the CO₂ injection shown an agreement within 10 % for most analytical species. The second step has been that to compute the geochemical impact of three years of CO₂ injection (September 2000-2003) by kinetically controlled reactions. In order to statically validated our geochemical model we have compared the computed and measured data by using the Median Test. The results show that the proposed geochemical model is able to reliably describe (within 5% error) the behaviour of pH, HCO₃, Cl, Li, Na, Sr, Si and HS+SO₄, with the exception of K, Ca and Mg. Finally, the kinetic evolution of the CO₂-rich Weyburn brines interacting with the host-rock minerals, performed over 100 years after injection, has also been modelled. The solubility trapping (short/medium-term sequestration) gives an amount of dissolved CO2 of 0.761moles/L and 0.752 moles/L for Marly and Vuggy units, respectively, whereas the mineral trapping, calculated as difference between dissolved (calcite and dolomite) and precipitated carbonate (dawsonite) minerals, is -0.019 and -5.69x10⁻⁵ moles/L for Marly and Vuggy units, respectively. The experimental data-set available and the geochemical modelling intrinsic limitation introduce a large uncertainty in the modelled results and in order to evaluate the dependence of the results from the modeling code, a different thermodynamic approach, such as the modelling software GEM (Gibbs Energy Minimization approach), is required.