



## 2D reactive transport simulations of CO<sub>2</sub> flue gas containing impurities in a saline aquifer, Heletz, Israel

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The impact of impurities in CO<sub>2</sub> flue gas within the carbon dioxide capture and storage chain grew in attention in recent years. From a techno-economical perspective it is desirable to leave impurities like N<sub>2</sub>, Ar, O<sub>2</sub>, SO<sub>x</sub>, NO<sub>x</sub>, or H<sub>2</sub> from the industrial CO<sub>2</sub> sources in the compressed gas stream to save cleaning costs during the capture operations. At the same time upper concentration limits for these impurities are under discussion to ensure a least-corrosive pipeline transport, justifiable compression work and safe injection and storage operations in geological reservoirs like saline aquifers without distinct alteration of the prevailing rock properties and mineral phase compositions.

In the framework of the EU funded CO<sub>2</sub>QUEST project, numerical 2D reactive transport simulations of impure CO<sub>2</sub> injection containing SO<sub>2</sub> and NO<sub>2</sub> into a saline aquifer were performed. Here, the common simulation code TOUGHREACT V3.0-OMP was used. The goal of this work was to determine the impact of co-injected impurities on the geochemical system of the storage aquifer and its mineral phases in order to curtail the potential impurity induced changes on a reservoir scale.

Special emphasis was given on the interaction between reactive dynamics of the impurities dissolved in the aqueous phase with the mineral phases and the hydraulic transport properties of the CO<sub>2</sub>-rich and aqueous phases. Thus it was possible to determine the spatial extent and the qualitative and quantitative degree of mineral alteration caused by co-injected impurities during CO<sub>2</sub> injection.

A prominent feature of the results of these simulations can be described as “chromatographic separation” of the impurities during the transport movement of the CO<sub>2</sub> phase. Due to the preferential dissolution of SO<sub>2</sub> and NO<sub>2</sub> into the aqueous phase compared to CO<sub>2</sub>, the CO<sub>2</sub> phase is depleted of these impurities during the outwards spreading movement given a sufficiently large interface area to the aqueous phase. Hence, the reservoir volume characterised by highly concentrated dissolved impurities and their impact on reservoir rock minerals is much more restricted in its spatial extent compared to the dimension of the whole CO<sub>2</sub> plume. For our set of initial conditions (pressure, temperature, salinity, injection rate and duration, reservoir height, initial porosity and permeability) the geochemical impact of SO<sub>2</sub> and NO<sub>2</sub> is limited to 250 m or less in radial distance (depending of the height  $z$ ), while the whole CO<sub>2</sub> plume reaches a maximum extent of approximately 2200 m directly below the upper lying caprock layer.

Within this “area of impurity impact” the geochemical response of the near equilibrium sandstone aquifer on the disturbance by highly acidic and redox sensitive impurities is dominated by the buffering dissolution of available carbonate phases and the reprecipitation of Ca<sup>2+</sup> containing sulfate

phases, i.e. anhydrite. The presence of dissolved  $\text{NO}_2$  leads to a local redox imbalance, whereby mainly ferrous iron ( $\text{Fe}^{2+}$ ) containing minerals dissolve and ferric iron ( $\text{Fe}^{3+}$ ) oxides precipitate. Generally it can be stated that the relatively small fractions of impurities cause more intense mineral dissolution and precipitation reactions locally compared to pure  $\text{CO}_2$ , whereas a slight porosity increase can be predicted in this case, see Figure 1. However, this strongly depends on the availability and the type of prevailing carbonate phases and thus has to be evaluated for each single reservoir under consideration for utilisation in CCS projects.

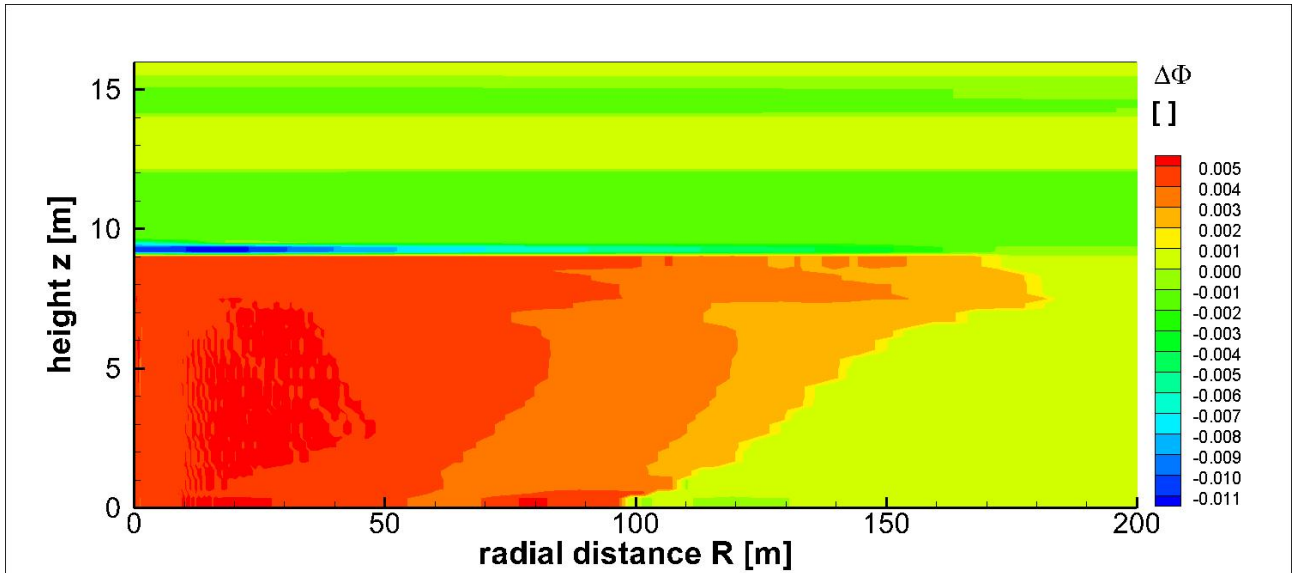


Figure 1: 2D spatial distribution of the change of porosity  $\Delta\Phi$  after ten years of  $\text{CO}_2$  injection including 1 %  $\text{SO}_2$ . The porosity increase (orange to red area) on the first 9 m of height and up to 180 m in radial distance corresponds to the rock volume impacted by dissolved  $\text{SO}_2$ . The above located layers are protected from  $\text{SO}_2$  due to a sealing intermediate shale layer from 9 m to 11 m in height.