Carbonate/Clays Reactions as source of CO_2 natural accumulations: quantification and propagation of uncertainties in modelling of CO_2 generation in sedimentary basins

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We present a methodological framework to model CO_2 generation by Carbonate/Clays Reactions (CCR) in large-scale subsurface systems under multiple sources of uncertainty. Our approach couples a one-dimensional compaction model, providing the dynamics of the evolution of porosity, temperature and pressure along the vertical direction, with a chemical model, describing the postulated interactions between mineral phases and fluid phases along the depth. This modeling framework allows (*i*) estimating the depth at which the source of gasses is located; and (*ii*) quantifying the amount of CO_2 generated according to different feasible CCR mechanisms in the basin formation process. A distinctive objective of the study is to provide a procedure for the quantification of the uncertainty affecting chemical equilibrium constants and to propagate the effect of the uncertainty to model output, i.e. CO_2 generation. We consider these parameters as key sources of uncertainty in geochemical modeling, as temperature and pressure associated with deeply buried sediments generally fall outside the range of validity of commonly employed geochemical databases. As a test bed, we consider a case study representative of a realistic sedimentary formation. Our results are conducive to the probabilistic assessment of (*i*) the relevance of CCR in the generation of CO_2 under realistic conditions of temperature and pressure in sedimentary environments, and (*ii*) the characteristic pressure and temperature at which CCR leads to the generation of CO_2 in sedimentary systems. Finally, we compare the sensitivity of CO_2 generation to thermochemical uncertainties against other possible sources of uncertainty affecting thermal/diagenetic evolution of basin in our model procedure.