Quantification of CO$_2$ generation in sedimentary basins through Carbonate/Clays Reactions with uncertain thermodynamic parameters

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Abstract

We develop a methodological framework and mathematical formulation which yields (i) characterization of the main features of carbonate-clays reactions (CCR) and (ii) estimates of the uncertainty associated with the amounts of $CO_2$ generated by this geochemical process in large-scale subsurface systems. 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, characterizing the set of key chemical reactions describing the postulated interactions between mineral phases and water along depth. This modeling framework allows (i) identifying the relative contribution of the mechanisms involved in the analysis within a given sedimentary basin; (ii) estimating the depth at which the source of gases is located; and (iii) quantifying the amount of $CO_2$ generated, based on the mineralogy of the sediments involved in the basin formation process. A distinctive objective of the study is the quantification of the way the uncertainty affecting chemical equilibrium constants propagates to model outputs, i.e., the flux of $CO_2$. These parameters are considered as key sources of uncertainty in our modeling approach because temperature and pressure distributions associated with deep burial depths typically fall outside the range of validity of commonly employed geochemical databases. We also analyze the impact of the mineralogy of the sediments on the activation of CCR processes. 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, and (ii) the characteristic pressure and temperature at which CCR leads to generation of $CO_2$ in sedimentary systems.