

Introduction

Secondary migration transports hydrocarbon from source rocks to a reservoir through permeable carrier rocks. Organic catagenesis byproducts (e.g., CO₂, H₂S, and organic acids) and carbonic acid and carboxylic acids generated from oil degradation are corrosive to the carrier and reservoir rocks. The interactions between these acidic components and inorganic chemicals—solutes in brine and minerals in the solid matrix—can increase or redistribute the porosity and facilitate the creation of exploration “sweet spots.” However, controversy exists as to whether these interactions occur at a scale that is truly significant to reservoir quality and petroleum accumulation.

Much of this controversy centers on the plausibility of mass balance and thermodynamics. **Coupled Reactive Transport Modeling (RTM)** is effective to address these two key constraints, *quantitatively*. In this study, we use RTMs to simulate the multiphase flow of gas and water through a carrier bed and into a reservoir along temperature and pressure gradients at a time and spatial scales of up to 10⁶ – 10⁷ years and 10² kilometers, respectively, and test many concepts, arguments, and assumptions through scenarios analysis.

Figure 1. Evolution of porosity in the simulation domain at (A) 5 Ma and (C) 15 Ma. (E) is the enlarged view of porosity distribution in the gas trap at 20 Ma, showing the position of Profiles 1 and 2. Due to artificial errors in modeling boundaries, anomaly porosity increases are observed near the left and right boundaries (A and C); however, the anomalies are limited to near the boundaries and do not propagate upward.

Progress to date

Basin-scale coupled reactive transport modeling

Numerical models for the charging of natural gas rich in acidic components (CO₂) were developed for generic carbonate and sandstone reservoirs, respectively, to answer the following questions: (1) Can acidic matter redistribute/modify the local pores of reservoirs at a large scale? (2) How does the dissolved mass migrate? (3) What is the degree of local porosity change? (4) Dissolution/precipitation of which mineral(s) control(s) porosity redistribution/modification?

For the carbonate reservoir, simulation results (Fig. 1) indicate (1) CO₂ can induce local mesogenetic dissolution, which occurs mainly in the vicinity of gas-water-contact (GWC) and, for the configuration in this study, results in the porosity increase limited in the trap. The dissolved minerals are transferred out by the groundwater flow. (2) Mesogenetic dissolution occurs on the localized area in the formation (e.g., the trap), not the entire formation. Therefore, it only requires a small amount of CO₂ and groundwater. The limited CO₂ from source rock and groundwater flow in the subsurface seem to be sufficient to support local secondary porosity generation.

A Mineral-Water-Gas Interaction Model of $p\text{CO}_2$ as a Function of Temperature in Sedimentary Basins

Accurate prediction of CO₂ partial pressure ($p\text{CO}_2$) in sedimentary basins is important for reducing the risks in natural gas exploration, improving reservoir quality prediction, optimizing production and reservoir management operations and understanding of geological storage of CO₂. We developed a holistic model of CO₂-water-rock interactions to interpret and predict $p\text{CO}_2$ in sedimentary basins. This improved model considers a gas phase explicitly, the gas composition through a Peng-Robinson equation of state, the pressure effects on thermodynamic properties of minerals and aqueous species, an expanded mineral assemblage, and the basin re-subsidence history. $p\text{CO}_2$ values under these conditions was then calculated via reaction path modeling.

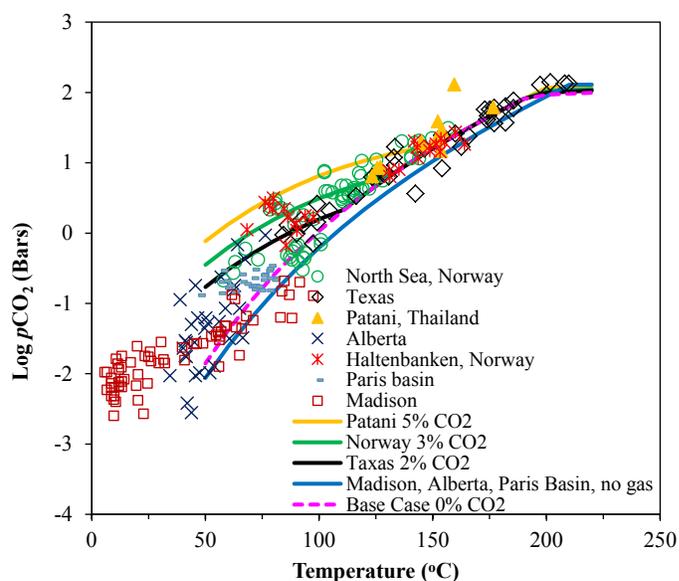


Figure 2. $\log(p\text{CO}_2)$ as a function of temperature (and the corresponding pressure) in sedimentary basins with a simple burial history (monotonic subsidence). Symbols are field data and lines are simulation results.

The modeling results indicated that $p\text{CO}_2$ values in the sedimentary basin as a function of temperature are controlled not only by the thermodynamic equilibrium between water and aluminosilicate and carbonate minerals but also by the availability and composition of the co-existing initial gas (Fig 2). The effects of the addition of the same percentage of gas impurities on the $\log(p\text{CO}_2)$ values in an increased order are H₂, N₂, H₂S, and CO₂. Different mineral compositions in the initial mineral assemblage would affect the mineral buffering capacity of the system.

Timeline to completion

Model development occurred in Year 1. During Year 2, Tasks 4-5 will be performed (Task 4: Influence of regional groundwater flow; Task 5: Influence of organic acids on the dissolution kinetics of aluminosilicate minerals). Presentations of results will be made at national meetings (e.g. AAPG, ACS, and SPE) during Year 2. Results will then be submitted to peer-reviewed journals for publication. The Ph.D. student is expected to graduate.

Impact of Research

The research supported by this ACS-PRF New Direction grant represents a significant step forward in our understanding of the organic-inorganic interactions (water-gas-rock-hydrocarbon integrations) during hydrocarbon migration. The support provided to one graduate student has allowed him to continue his research into thermodynamics and kinetics of geochemical reactions, which forms the core of the student's Ph.D. dissertation.

Publications

(‡student authors; *corresponding authors)

Lu P, Luo P, ‡Zhang GR, Zhang S, *Zhu C. An Improved Model of $p\text{CO}_2$ as a Function of Temperature in Sedimentary Basins. (To be submitted to *Geology*)

‡Zhang GR, Lu P, *Zhu C (accepted) Effects of natural gas acidic components on local porosity generation in a carbonate reservoir: Insights from reactive transport modeling. AAPG Bulletin.